THREE-DIMENSIONAL STRUCTURE OF COMPLEMENT RECEPTOR TYPE 2 AND USES THEREOF

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Field of the Invention

This invention relates to the crystallization and resolution of the three-dimensional structure of the human complement receptor type 2 (CR2) protein, and to methods of using such structure, particularly for structure-based drug design of regulatory compounds.

Background of the Invention

Complement receptor type 2 (CR2 or CD21) is a key interface between innate and adaptive immunity by serving as the receptor for complement component C3d, as well as for C3 and fragments of C3 that contain the C3d domain or a portion thereof, including but not limited to C3dg, iC3b and C3b (D. T. Fearon and R. H. Carter, *Annu Rev Immunol* 13, 127-49 (1995); D. T. Fearon, *Semin Immunol* 10, 355-61 (1998)). C3d and other CR2-binding C3 fragments that contain C3d or a portion thereof are covalently attached to foreign antigens (such as invading microorganisms) through the action of the classical, alternative or lectin complement pathways (S. K. A. Law and K. B. M. Reid, *Complement,*. D. Male, Ed., In Focus (Oxford, UK:IRL Press., ed. second edition, 1995)). C3d- or other CR2-binding C3 fragment-bound antigens then greatly amplify B cell responses by binding to CR2 through these C3 fragments at the same time as engaging the B cell receptor (BCR) via the bound antigen (R. H. Carter and D. T. Fearon, *Science* 256, 105-7 (1992); J. C. Cambier, *Biochem Soc Trans* 25, 441-5 (1997)). The cross-linking of CR2 to the BCR by C3d, C3, or other CR2-binding fragments of C3 that contain C3d or a portion thereof greatly amplifies a signal transduction cascade through the CR2/CD19/CD81 co-activation complex (D. T. Fearon,

1995 *ibid.*; D. T. Fearon, 1998, *ibid.*; J. C. Cambier, 1997, *ibid.*; A. K. Matsumoto, et al., *J Exp Med* 173, 55-64 (1991)).

Human CR2 is also the obligate receptor for the Epstein-Barr virus (EBV) through its interactions with the gp350/220 viral membrane protein (J. D. Fingeroth, et al., *Proc Natl Acad Sci USA* 81, 4510-4 (1984)). EBV causes infectious mononucleosis, and is associated with Burkitt's Lymphoma and several other lymphomas and non-lymphoid tumors (M. Okano, *Acta Paediatr* 87, 11-8 (1998)). In addition, human CR2 serves as a receptor for CD23 (J. P. Aubry et al., *Nature* 358, 505-7 (1992)) and is thus a receptor for at least three biologically important ligands. Using genetically manipulated mice and animal models, CR2 has been shown to be essential for the development of normal humoral immunity to T-dependent antigens (T. Hebell et al., *Science* 254, 102-5 (1991); J. M. Ahearn, et al., *Immunity* 4, 251-62 (1996); H. Molina, et al., *Proc Natl Acad Sci USA* 93, 3357-61 (1996)) as well as possibly play an important role in the maintenance of B cell self-tolerance and the development of autoimmunity (A. P. Prodeus, et al., *Immunity* 9, 721-31 (1998)). CR2 has also been shown to mediate the interaction of C3-bound HIV-1 as an immune complex with B cells in a fashion that promotes transfer of virus and infection of CD4 T cells (S. Moir, et al., *J Exp Med* 192, 637-46 (2000)). CR2 also mediates direct infection of CR2-expressing T cells or other CR2-expressing cell lineages that are bound by HIV-1 immune complexes containing C3, C3d or other CR2-binding C3 fragments (including, but not limited to, HIV-1 complexed with C3d).

Interactions with all three human CR2 ligands require the first two of 15 or 16 short consensus repeat (SCR) domains (C. A. Lowell, et al., *J Exp Med* 170, 1931-46 (1989); J. C. Carel et al., *J Biol Chem* 265, 12293-9 (1990)). SCR domains, like Ig domains, are found in many proteins from both complement and non-complement families, and mediate diverse biological functions (A. P. Wiles, et al., *J Mol Biol* 272, 253-65 (1997)). Several of the SCR proteins also serve as receptors for important human pathogens. For example, in addition to CR2, CD46 is a Measles Virus receptor (R. E. Dorig et al., *Cell* 75, 295-305 (1993)), and

CD55 is an echovirus receptor (T. Ward, et al., *EMBO J* 13, 5070-4 (1994); J. M. Bergelson, et al., *Proc Natl Acad Sci U S A* 91, 6245-9 (1994)). Previously determined structures of SCR proteins containing two or four SCR domains have revealed a conserved core structure but variable orientations between domains mediated in part by relatively short 3-8 amino acid inter-SCR linker peptides (A. P. Wiles, et al., 1997, *ibid.*; P. N. Barlow, et al., *J Mol Biol* 232, 268-84 (1993); J. M. Casasnovas et al., *EMBO J* 18, 2911-22 (1999); R. Schwarzenbacher, et al., *EMBO J* 18, 6228-39 (1999)). As one of the major functions of SCR domains is to mediate protein-protein (such as receptor-ligand) interactions, and at least two SCRs have been found to be required for these interactions, the relative angle and orientation unique to each SCR-containing protein is likely to contribute to both biologic diversity as well as specificity. However, the lack of a high-resolution structure of a receptor-ligand complex in this family has hindered the understanding of the molecular recognition mechanisms of this class of proteins. With regard to the structure of CR2 and the molecular interactions with its ligands, C3d and EBVgp350/220, variable results have been obtained using mutagenesis, monoclonal antibody, and peptide strategies (C. A. Lowell, et al., *J Exp Med* 170, 1931-46 (1989); D. R. Martin et al., *J Exp Med* 174, 1299-311 (1991); H. Molina, et al., *J Biol Chem* 266, 12173-9 (1991); H. Molina et al., *J Immunol* 153, 789-95 (1994); D. R. Martin et al., *J Virol* 68, 4716-26 (1994); H. Molina, et al., *J Immunol* 154, 5426-35 (1995)).

Therefore, there is a need in the art for a three dimensional structure of CR2 in order to better understand the molecular recognition mechanisms of the protein and to enable the identification and/or design of compounds that mimic, enhance, disrupt or compete with the interactions of CR2 with its ligands.

Summary of the Invention

One embodiment of the present invention relates to a method of structure-based identification of compounds which potentially bind to complement receptor type 2 (CR2)

proteins or to a complex of CR2 and its ligand. This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region; and, (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a). The three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region is selected from: (i) a structure defined by atomic coordinates of a three dimensional structure of a crystalline CR2 SCR1-2 region in complex with C3d; (ii) a structure defined by atomic coordinates selected from: (1) atomic coordinates represented in a table selected from the group consisting of Table 2 (CR2-C3d) and Table 3 (CR2 only); and, (2) atomic coordinates that define a three dimensional structure, wherein at least 50% of the structure has an average root-mean-square deviation (RMSD) from backbone atoms in secondary structure elements in at least one domain of a three dimensional structure represented by the atomic coordinates of (1) of equal to or less than about 1.0Å; and (ii) a structure defined by atomic coordinates derived from CR2 protein molecules arranged in a crystalline manner in a space group R32 so as to form a unit cell of dimensions a=b=170.5Å, c=173.8 Å.

In one aspect of this embodiment, the step of identifying comprises selecting candidate compounds that potentially bind to and activate CR2.

In another aspect of this embodiment, the method further includes the step of: (c) selecting candidate compounds of (b) that inhibit the binding of CR2 to its ligand. The step (c) of selecting can include: (i) contacting the candidate compound identified in step (b) with CR2 or a fragment thereof and a CR2 ligand or a fragment thereof under conditions in which a CR2-CR2 ligand complex can form in the absence of the candidate compound; and (ii) measuring the binding affinity of the CR2 or fragment thereof to the CR2 ligand or fragment thereof; wherein a candidate inhibitor compound is selected as a compound that inhibits the binding of CR2 to its ligand when there is a decrease in the binding affinity of the CR2 or fragment thereof for the CR2 ligand or fragment thereof, as compared to in the absence of the candidate inhibitor compound. The CR2 ligand can include, but is not limited to, C3d,

C3, a CR2-binding fragment of C3 containing C3d, CD23, and Epstein Barr Virus (EBV) gp350/220, or CR2-binding fragments of any of the ligands. In one aspect, the CR2 protein or fragment thereof comprises an amino acid sequence selected from the group of SEQ ID NO:4 and SEQ ID NO:6.

In another aspect of this embodiment, the method further includes the step of: (c) selecting candidate compounds that stabilizes a complex of CR2 with its ligand. Step (c) can include: (i) contacting the candidate compound identified in step (b) with a CR2-CR2 ligand complex, wherein the CR2-CR2 ligand complex comprises CR2 or a fragment thereof and a CR2 ligand, or a fragment thereof; and (ii) measuring the stability of the CR2-CR2 ligand complex of (i), wherein a candidate stabilizer compound is selected as a compound that stabilizes the CR2-CR2 ligand complex when there is an increase in the stability of the complex as compared to in the absence of the candidate stabilizer compound. In this aspect, the ligand is preferably selected from C3d, C3, a CR2-binding fragment of C3 containing C3d, CD23, and CR2-binding fragments of any of the ligands. In this aspect, the CR2 protein or fragment thereof can comprise an amino acid sequence selected from the group of SEQ ID NO:4 and SEQ ID NO:6.

In the method of identifying a compound, the step (a) of identifying can include identifying candidate compounds for binding to the SCR2 domain of the CR2. In one aspect, the step of identifying includes identifying candidate compounds for binding to the interface between the SCR1 and SCR2 domains of CR2. In another aspect, the step of identifying includes identifying candidate compounds for binding to the dimer interface between two CR2 proteins. In yet another aspect, the step of identifying includes identifying candidate compounds for binding to the interface between CR2 and C3d, C3, a CR2-binding fragment of C3 containing C3d, or a fragment thereof. In one aspect, the step of identifying includes identifying candidate compounds for binding to the B strand and the B-C loop of CR2 SCR2 comprising the segment: G79-G80-Y81-K82-I83-R84-G85-S86-T87-P88-Y89. In another aspect, the step of identifying includes identifying candidate compounds for binding to a site

on the B strand of CR2 SCR2 comprising position K100. In another aspect, the step of identifying includes identifying candidate compounds for binding to a segment of CR2 SCR2 comprising V130-F131-P132-L133. In yet another aspect, the step of identifying comprises identifying candidate compounds for binding to a segment of CR2 SCR2 comprising the fragment T101-N102-F103. In one aspect of the method of identifying, the step of identifying includes identifying candidate compounds for binding to amino acid residues at positions 84 and 86 of an amino acid sequence selected from the group consisting of SEQ ID NO:4 and SEQ ID NO:6.

When the ligand is C3d, C3, or a CR2-binding fragment of C3 containing C3d, the step of identifying can include identifying candidate compounds for binding to the loop between helix 2-3 of C3d comprising the segment Q68-P69-S70-S71. In another aspect, the step of identifying can include identifying candidate compounds for binding to Helix 5 of C3d comprising the segment S104-Q105-V106-L107-C108-G109-A110-V111-K112-W113-L114-I115-L116-E117-K118-Q119-K120-P121-D122. In another aspect, the step of identifying can include identifying candidate compounds for binding to Helix 7of C3d comprising the segment N170-S171-L172-P173-G174-S175-I176-T177-K178-A179-G180-D181-F182-L183-E184-A185.

The step of identifying a compound in the method of the present invention can include any suitable method of drug design, drug screening or identification, including, but not limited to: directed drug design, random drug design, grid-based drug design, and/or computational screening of one or more databases of chemical compounds.

Yet another embodiment of the present invention relates to a method to identify a compound that inhibits the complement receptor type 2 (CR2)-dependent infection of a host cell by Epstein Barr Virus (EBV). This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound

structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a cell that expresses CR2 or a ligand binding fragment thereof and an Epstein Barr Virus (EBV) particle under conditions in which the EBV particle can bind to CR2 and infect the cell in the absence of the candidate compound; and (d) measuring the intracellular EBV titer of the cell; wherein a candidate inhibitor compound is selected as a compound that inhibits the EBV titer in the cell, as compared to in the absence of the candidate inhibitor compound.

Yet another embodiment of the present invention relates to a method to identify a compound that inhibits the binding of CD23 to complement receptor type 2 (CR2). This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a first cell expressing CR2 or a ligand binding fragment thereof and a second cell expressing a CD23 protein or fragment thereof under conditions in which the CD23 protein or fragment thereof and the CR2 or the ligand binding fragment thereof can bind in the absence of the candidate compound; and (d) measuring a biological activity induced by the interaction of CD23 and CR2 in the first or second cell; wherein a candidate inhibitor compound is selected as a compound that inhibits the biological activity as compared to in the absence of the candidate inhibitor compound. In a preferred embodiment, the biological activity is IgE isotype switching in the first cell.

Yet another embodiment of the present invention relates to a method to identify a compound that inhibits the binding of C3d, C3 or another CR2-binding fragment of C3 containing C3d or a portion thereof, to complement receptor type 2 (CR2). This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) identifying a candidate compound

for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a cell expressing CR2 or a fragment thereof and C3d, C3, a CR2-binding fragment of C3 containing C3d, or a fragment thereof, under conditions in which the C3d, the C3, the CR2-binding fragment of C3 containing C3d, or a fragment thereof, can bind to CR2 or the fragment thereof and enhance cell activation in the absence of the candidate compound; and (d) measuring the activation of the cell; wherein a candidate inhibitor compound is selected as a compound that inhibits cell activation, as compared to in the absence of the candidate inhibitor compound. In this embodiment, the cell in (c) can include, but is not limited to: a B cell, a T cell, a thymocyte, an epithelial cell, and a mast cell. Activation can be measured by any suitable method including, but not limited to: measurement of cytokine production by the cell, measurement of calcium mobilization in the cell, measurement of lyn tyrosine kinase activity in the cell, measurement of phosphatidylinositol 3' kinase activity in the cell, measurement of activation of NF-κB, measurement of activation of MAP kinases, measurement of phosphorylation of CD19 in the cell, and measurement of activation of protein kinase C (PKC) in the cell.

Another embodiment of the present invention relates to a method to inhibit complement receptor type 2 (CR2)-dependent human immunodeficiency virus-1 (HIV-1) infection of cells in a patient. This method includes the steps of administering to a patient infected with HIV-1 an inhibitor compound that inhibits the binding of C3d, C3 or another CR2-binding fragment of C3 containing C3d or a portion thereof, -opsonized HIV-1 to B cells, follicular dendritic cells, T cells or macrophages in the patient. The inhibitor compound is selected by the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three

dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a B cell or follicular dendritic cell expressing CR2 or a fragment thereof and C3d, C3, a CR2-binding fragment of C3 containing C3d, or a fragment thereof, under conditions in which the C3d, the C3, the CR2-binding fragment of C3 containing C3d, or the fragment thereof, can bind to CR2 and enhance B cell activation or follicular dendritic cell activation in the absence of the candidate compound; and (d) measuring the activation of the B cell or the follicular dendritic cell, wherein a candidate inhibitor compound is selected as a compound that inhibits B cell activation or follicular dendritic cell activation, as compared to in the absence of the candidate inhibitor compound.

Yet another embodiment of the present invention relates to a method to prepare a vaccine. This method includes linking a compound that increases B cell activation to an antigen to form the vaccine, wherein the compound is selected by the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a B cell expressing CR2 or a fragment thereof and with C3d, C3, a CR2-binding fragment of C3 containing C3d, or a fragment thereof, under conditions in which the C3d, the C3, the CR2-binding fragment of C3 containing C3d, or the fragment thereof, can bind to and activate CR2 in the absence of the candidate compound; and (d) measuring the activation of the B cell; wherein a candidate compound for use in a vaccine is selected as a compound that increases B cell activation, as compared to in the absence of the candidate compound.

Yet another embodiment of the present invention relates to a drug delivery system, which includes: (a) a drug; and, (b) a portion of a CR2 protein selected from the group of: (i) positions on strand B and the B-C loop of SCR2 including: G79-G80-Y81-K82-I83-R84-G85-S86-T87-P88-Y89; (ii) position K100 on the B strand of CR2; and, (iii) positions:

V130-F131-P132-L133; and (iv) combinations of (i)-(iii). The drug is linked to the portion of CR2.

Yet another embodiment of the present invention relates to an antibody that selectively binds to CR2. The antibody binds to a portion of CR2 selected from the group of: (a) the interface between the SCR1 and SCR2 domains of CR2; (b) the dimer interface between two CR2 proteins; and, (c) the interface between CR2 and C3d. Preferably, an antibody that binds to an interface between CR2 and C3d selectively binds to a site selected from: (i) the B strand and the B-C loop of CR2 SCR2 comprising the segment: G79-G80-Y81-K82-I83-R84-G85-S86-T87-P88-Y89; (ii) the B strand of CR2 SCR2 comprising position K100; (iii) a segment of CR2 SCR2 comprising V130-F131-P132-L133; and, (iv) a segment of CR2 SCR2 comprising T101-N102-F103.

Yet another embodiment of the present invention relates to a crystal comprising complement receptor type 2 (CR2) in complex with C3d. The CR2 consists of SEQ ID NO:4, and the C3d consists of SEQ ID NO:7. The crystal effectively diffracts X-rays for the determination of the atomic coordinates of the CR2 in complex with C3d to a resolution of greater than 2.0 A, and the crystal has a space group R32 so as to form a unit cell of dimensions a=b=170.5Å, c=173.8 Å.

Another embodiment of the present invention is a therapeutic composition that, when administered to an animal, enhances B cell responses in the animal. The therapeutic composition comprises a compound that stimulates the activity of a complement receptor type 2 (CR2). The compound is identified by the method that includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) synthesizing the candidate compound; and (d) selecting candidate compounds that bind to and activate CR2.

Yet another embodiment relates to a therapeutic composition that, when administered to an animal, inhibits the biological activity of complement receptor type 2 (CR2) in the animal. The therapeutic composition includes a compound that inhibits the activity of a complement receptor type 2 (CR2). The compound is identified by the method that includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) synthesizing the candidate compound; and (d) selecting candidate compounds that inhibit the biological activity of CR2. Preferably, the compounds inhibit the formation of a complex between CR2 and a CR2 ligand. The ligand can include, C3d, C3, CR2-binding fragments of C3 containing C3d, CD23 and Epstein Barr Virus (EBV), and CR2-binding fragments any of the ligands. In one aspect, the compound inhibits the activation of CR2.

Yet another embodiment of the present invention relates to a method of preparing complement receptor type 2 (CR2) proteins having modified biological activity. This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described in detail above; (b) analyzing the three dimensional structure to the three-dimensional structure of the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify at least one site in the structure contributing to the biological activity of CR2; and (c) modifying the at least one site in a CR2 protein to alter the biological activity of the CR2 protein.

Yet another embodiment of the present invention relates to an isolated protein comprising a mutant C3d. The protein comprises an amino acid sequence that differs from SEQ ID NO:7 by an amino acid substitution selected from the group of: a non-asparagine amino acid residue at position 170, a non-isoleucine amino acid residue at position 115, and/or a non-leucine amino acid residue at position 116. The C3d mutant protein has

reduced binding to complement receptor type 2 (CR2), as compared to a wild-type C3d protein. In one aspect, the mutant protein comprises an amino acid sequence selected from the group consisting of SEQ ID NO:8 and SEQ ID NO:9.

Brief Description of the Drawings of the Invention

Fig. 1A shows an overall view of the structure of CR2 binding to C3d, showing only SCR2 contacting one portion of the edge of C3d.

Fig. 1B shows the overall structure showing a second CR2-C3d complex (colored in light blue and grey) that dimerizes with the first one in Fig. 1A.

Fig. 2A is a ribbon representation of the CR2 SCR1 (in red) and SCR2 (in yellow) structures, showing the SCR fold and the packing of the two domains to form a V shape.

Fig. 2B is a representation of the structure and packing interaction at the interface of CR2 SCR1 and SCR2 domains.

Fig. 2C is a surface representation of the two-domain arrangement of CR2.

Fig. 2D is a representation of the dimerization of CR2 through interactions between SCR1 of each molecule.

Fig. 2E is a sequence alignment between human CR2 (hCR2) SCR1-2 domains (SEQ ID NO:4) and mouse CR2 (mCR2) SCR1-2 domains (SEQ ID NO:6).

Figs. 3A and 3B are representations of the surface features of the interface area on C3d (in cyan) and CR2 molecule (in yellow).

Fig. 3C shows the structure of the CR2 SCR2-C3d complex.

Figs. 3D and 3E show the detailed interactions between CR2 (in yellow) and C3d (in cyan) in two angles.

Fig. 3F shows the human C3d sequence (SEQ ID NO:7) with secondary structure assigned on top of the corresponding sequences.

Fig. 4A is a digitized image of a native gel shift assay of the binding between CR2 and C3d wild type (wt) or mutants (mt).

Fig. 4B is a graphical representation showing the intensity changes of the complex bands (measured by densitometry) as CR2 concentration increases from lanes 2 to 4 (wt), or lanes 6 to 8 (mt115), or lanes 10 to 12 (mt170) in Fig. 4A.

Fig. 4C is a graphical representation of a competitive ELISA demonstrating the relative abilities of wild type versus mutant forms of C3d to block CR2-wild type C3d interactions.

Figs. 5A and 5B are two view with a 180 degree rotation to each other showing the localization of the epitopes of anti-CR2 monoclonal antibodies (mAb) on the CR2 surface.

Fig. 6A is a surface representation of the model containing a dimer of CR2 SCR1 and SCR2 that bind to C3d on each receptor.

Fig. 6B is a diagram of C3d-antigen cross-linking CR2 (as dimers) and BCR on the cell surface.

Detailed Description of the Invention

The present invention relates to the discovery of the three-dimensional structure of complement receptor 2 (CR2/CD21), to crystalline CR2-C3d complexes, to models of such three-dimensional structures, to a method of structure based drug design using such structures, to the compounds identified by such methods and to the use of such compounds in therapeutic compositions and methods. Complement receptor 2 (CR2/CD21) is an important receptor bridging the innate and adaptive immune systems that greatly amplifies B lymphocyte activation. CR2 ligands include complement C3d, C3, a CR-2 binding fragment of C3 that contains C3d or a portion thereof, CD23 and Epstein-Barr virus gp350/220. The structural basis for ligand binding by short consensus repeat (SCR) containing proteins has been unknown, but CR2 interactions require the presence of a two SCR-containing domain. In an effort to understand how CR2 interacts with its cellular ligand C3d in the process of B cell activation, as well as its other natural ligands, the present inventors have determined the 2 Å crystal structure of the CR2 SCR1 and SCR2 domain in

complex with C3d. The present inventors describe herein the x-ray structure of this CR2 domain in complex with C3d, which reveals extensive main chain interactions of C3d with one SCR of CR2 and substantial SCR side-side packing. These results provide the first detailed understanding of receptor-ligand interactions in this protein family and reveal potential target sites for molecular drug design.

According to the present invention, the complement receptor 2 (CR2/CD21) is a protein that is characterized by the amino acid sequence represented by SEQ ID NO:1. SEQ ID NO:1 represents the full-length human CR2 protein sequence. The two short consensus repeat (SCR) domains of CR2 that are known to be required for CR2-ligand interactions, SCR1 and SCR2, are located, respectively, within the human CR2 amino acid sequence between positions Cys23 and Cys82 (i.e., between the first Cys and the fourth Cys residues) of SEQ ID NO:1 (SCR1, also represented herein by SEQ ID NO:2) and between positions Cys91 and Cys146 (i.e., between the fifth Cys and the eighth Cys residues) of SEQ ID NO:1 (SCR2, also represented herein by SEQ ID NO:3). The segment (fragment) of human CR2 represented in crystal structure herein contains both the SCR1 and the SCR2 domain (positions 20-153 of SEQ ID NO:1), and is represented herein by SEQ ID NO:4. SEQ ID NO:4 includes the 8 residue linker between SCR1 (SEQ ID NO:2) and SCR2 (SEQ ID NO:3). It also contains three residues at the N-terminus of SCR1 that match exactly positions Gly20-Ser22 of SEQ ID NO:1. At the C-terminus of SCR2, SEQ ID NO:4 contains seven residues that match exactly positions Val147-Glu153 of SEQ ID NO:1.

The full-length mouse CR2 protein sequence is represented herein by SEQ ID NO:5. The SCR1 and SCR2 domains of the mouse CR2 protein are located with the mouse CR2 amino sequence at positions 14-73 of SEQ ID NO:5 (SCR1) and positions 82-138 of SEQ ID NO:5 (SCR2). The segment (fragment) of mouse CR2 that contains both the SCR1 and SCR2 domains and the eight residue linker, and which is shown aligned with the human sequence in Fig. 2E, is located at positions 11-145 of SEQ ID NO:5 and is represented herein by SEQ ID NO:6. Human and mouse CR2 are approximately 66% identical over the full

length amino acid sequences represented by SEQ ID NO:1 and SEQ ID NO:5 (using BLAST 2 pairwise alignment), and approximately 61% identical over the SCR1-SCR2 regions of SEQ ID NO:4 and SEQ ID NO:6 (using BLAST 2 pairwise alignment). It is noted that both mouse and human CR2 bind to C3 (in the C3d region).

According to the present invention, general reference to a complement receptor 2 (CR2/CD21) protein is a protein that, at a minimum, contains any portion of the SCR1 and SCR2 domains of a CR2 protein, and includes full-length CR2 proteins, soluble CR2 proteins, other biologically active fragments of CR2 proteins, CR2 proteins comprising SCR1 and SCR2, CR2 fusion proteins, or any homologue of a naturally occurring CR2, as described in detail below. A homologue of a CR2 protein includes proteins which differ from a naturally occurring CR2 in that at least one or a few, but not limited to one or a few, amino acids have been deleted (e.g., a truncated version of the protein, such as a peptide or fragment), inserted, inverted, substituted and/or derivatized (e.g., by glycosylation, phosphorylation, acetylation, myristoylation, prenylation, palmitation, amidation and/or addition of glycosylphosphatidyl inositol). Preferably, a CR2 homologue has an amino acid sequence that is at least about 70% identical to the amino acid sequence of a naturally occurring CR2 (e.g., SEQ ID NO:1, or SEQ ID NO:5), and more preferably, at least about 75%, and more preferably, at least about 80%, and more preferably, at least about 85%, and more preferably, at least about 90%, and more preferably, at least about 95% identical to the amino acid sequence of a naturally occurring CR2. Preferred three-dimensional structural homologues of a CR2 are described in detail below. According to the present invention, a CR2 homologue preferably has, at a minimum, the ability to bind to a naturally occurring ligand of CR2 (e.g., C3d (including any C3 fragments with CR2-binding ability), CD23, EBV). Such homologues include fragments of a full length CR2 (e.g., the SCR2 region or the SCR1-SCR2 region) and can be referred to herein as a CR2 ligand-binding fragment. In one embodiment, a CR2 homologue has the biological activity of a naturally occurring CR2. Reference to a CR2 protein can also generally refer to CR2 in complex with a ligand.

In general, the biological activity or biological action of a protein refers to any function(s) exhibited or performed by the protein that is ascribed to the naturally occurring form of the protein as measured or observed *in vivo* (i.e., in the natural physiological environment of the protein) or *in vitro* (i.e., under laboratory conditions). Modifications of a protein, such as in a homologue or mimetic (discussed below), may result in proteins having the same biological activity as the naturally occurring protein, or in proteins having decreased or increased biological activity as compared to the naturally occurring protein. Modifications which result in a decrease in protein expression or a decrease in the activity of the protein, can be referred to as inactivation (complete or partial), down-regulation, or decreased action of a protein. Similarly, modifications which result in an increase in protein expression or an increase in the activity of the protein, can be referred to as amplification, overproduction, activation, enhancement, up-regulation or increased action of a protein. As used herein, a protein that has "CR2 biological activity" or that is referred to as a CR2 refers to a protein that has an activity that can include any one, and preferably more than one, of the following characteristics: (a) binds to a natural ligand of CR2 (e.g., C3d, EBV, CD23, C3 or other CR2-binding C3 fragments); (b) mediates interactions between the natural ligands and other proteins; (c) responds to contact with a natural ligand or other agonist (i.e., stimulation) by activation of the signal transduction cascade through the CR2/CD19/CD81 co-activation complex in a cell expressing such complex (D. T. Fearon, 1995 *ibid.*; D. T. Fearon, 1998, *ibid.*; J. C. Cambier, 1997, *ibid.*; A. K. Matsumoto, et al., *J Exp Med* 173, 55-64 (1991)), including activation of lyn tyrosine kinase, activations of phosphatidyl inositol 3' kinase, activation of NF-κB, activation of MAP kinases, phosphorylation of CD19, activation of PI3 kinase, and activation of protein kinase C (PKC). Such biological activities of (c) associated with the binding and activation of CR2 can be referred to as downstream biological activities, since they occur downstream of the binding of CR2 by its ligand.

An isolated protein (e.g., an isolated CR2 protein or an isolated C3d protein, an isolated C3 protein, or other CR2-binding C3 fragment), according to the present invention,

is a protein that has been removed from its natural milieu (i.e., that has been subject to human manipulation) and can include purified proteins, partially purified proteins, recombinantly produced proteins, and synthetically produced proteins, for example. As such, "isolated" does not reflect the extent to which the protein has been purified. Preferably, an isolated protein, and particularly, an isolated CR2 protein and/or an isolated C3d protein or other CR2-binding C3 fragment, is produced recombinantly. According to the present invention, a CR2-binding C3 fragment can include any portion of C3 that contains at least a portion of C3d sufficient to bind to CR2, and can include, but is not limited to, portions of C3 comprising C3dg, iC3b, and/or C3b, an isolated C3d segment or a portion thereof. The terms "fragment", "segment" and "portion" can be used interchangeably herein with regard to referencing a part of a protein.

Reference to a protein from a specific organism, such as a "human CR2", by way of example, refers to a CR2 (including a homologue of a naturally occurring CR2) from a human or a CR2 protein that has been otherwise produced from the knowledge of the primary structure (e.g., sequence) and/or the tertiary structure of a naturally occurring CR2 protein from a human. In other words, a human CR2 protein includes any CR2 protein that has the structure and function of a naturally occurring CR2 protein from a human or that has a structure and function that is sufficiently similar to a human CR2 protein such that the CR2 protein is a biologically active (i.e., has biological activity) homologue of a naturally occurring CR2 protein from a human. As such, a human CR2 protein can include purified, partially purified, recombinant, mutated/modified and synthetic proteins.

Proteins of the present invention are preferably retrieved, obtained, and/or used in "substantially pure" form. As used herein, "substantially pure" refers to a purity that allows for the effective use of the protein *in vitro*, *ex vivo* or *in vivo* according to the present invention. For a protein to be useful in an *in vitro*, *ex vivo* or *in vivo* method according to the present invention, it is substantially free of contaminants, other proteins and/or chemicals that might interfere or that would interfere with its use in a method disclosed by the present

invention, or that at least would be undesirable for inclusion with the protein when it is used in a method disclosed by the present invention. For example, for a CR2 protein, such methods include crystallization of the protein, use of a portion of the protein as a drug delivery vehicle, antibody production, agonist/antagonist identification assays, and all other methods disclosed herein. Preferably, a "substantially pure" protein, as referenced herein, is a protein that can be produced by any method (i.e., by direct purification from a natural source, recombinantly, or synthetically), and that has been purified from other protein components such that the protein comprises at least about 80% weight/weight of the total protein in a given composition (e.g., the protein is about 80% of the protein in a solution/composition/buffer), and more preferably, at least about 85%, and more preferably at least about 90%, and more preferably at least about 91%, and more preferably at least about 92%, and more preferably at least about 93%, and more preferably at least about 94%, and more preferably at least about 95%, and more preferably at least about 96%, and more preferably at least about 97%, and more preferably at least about 98%, and more preferably at least about 99%, weight/weight of the total protein in a given composition.

As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute the protein. The "three dimensional structure" or "tertiary structure" of the protein refers to the arrangement of the components of the protein in three dimensions. Such term is well known to those of skill in the art. It is also to be noted that the terms "tertiary" and "three dimensional" can be used interchangeably.

The present invention provides the atomic coordinates that define the three dimensional structure of a CR2 protein in complex with a C3d protein. A CR2-ligand complex, such as a CR2-C3d complex, refers to the complex (e.g., interaction, binding), that forms between CR2 and any of its ligands (e.g., C3d) in the absence of a compound that interferes with the interaction between the CR2 and its ligand(s). A complex is naturally formed between at least one full length CR2 and a full length ligand, but according to the

present invention, a CR2-ligand can also include complexes that minimally contain: (1) a CR2 SCR1 and/or CR2 SCR2 domain; and (2) a CR2-contacting portion of a ligand of CR2.

One embodiment of the present invention includes a CR2 protein in crystalline form. The present invention specifically exemplifies a portion of CR2 comprising the SCR1 and SCR2 domains. As used herein, the terms "crystalline CR2" and "CR2 crystal" both refer to crystallized CR2 protein and are intended to be used interchangeably. Preferably, a crystalline CR2 is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 1. A CR2 crystal of the present invention can comprise any crystal structure and preferably crystallizes as an orthorhombic crystal lattice. A suitable crystalline CR2 of the present invention includes a monomer or a dimer, or a multimer of CR2 protein. One preferred crystalline CR2 comprises between one and five CR2 proteins in an asymmetric unit. A more preferred crystalline CR2 comprises a dimer of CR2 proteins. Preferably, a composition of the present invention includes CR2 protein molecules arranged in a crystalline manner in a space group R3 or R32 so as to form a unit cell of dimensions a=b=170.5Å, c=173.8 Å. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates of the CR2 protein to a resolution of about 4.0 Å, and preferably to about 3.0 Å, and more preferably to about 2.0 Å.

One embodiment of the present invention includes a method for producing crystals of CR2, alone or in complex with a CR2 ligand, comprising combining CR2 protein with a mother liquor and inducing crystal formation to produce the CR2 crystals. Although the production of crystals of CR2 in complex with C3d are specifically described herein, it is to be understood that such processes as are described herein can be adapted by those of skill in the art to produce crystals of CR2 in complex with other CR2 ligands, such as Epstein Barr Virus (EBV) or CD23.

By way of example, crystals of CR2 and C3d in complex are formed using a solution containing about 20 mg/ml of CR2-C3d complex in a mother liquor. A suitable mother

liquor of the present invention comprises an acetate buffer or a sulfate buffer. A preferred acetate buffer of the present invention comprises zinc acetate or zinc sulfate. The concentration of ammonium acetate in the buffer prior to crystallization is preferably 0.2M. The pH of the acetate buffer (pH 7.36) is controlled using 0.1 M NaCacodylate. The acetate buffer also contains any polyethylene glycol (PEG), with PEG 2000 at a concentration of about 17% being more preferred. Supersaturated solutions of CR2-C3d complex can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of CR2-C3d complex are induced to crystallize by hanging drop vapor diffusion. In a vapor diffusion method, a CR2-C3d complex is combined with a mother liquor of the present invention that will cause the CR2-C3d complex solution to become supersaturated and form CR2-C3d complex crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature and, by way of example, can be performed at 4° C.

One embodiment of the present invention includes a representation, or model, of the three dimensional structure of a CR2 protein, such as a computer model. A computer model of the present invention can be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Heleneborgsgatan 21C, SE-11731 Stockholm, Sweden), the graphical display program O (Jones et. al., *Acta Crystallography*, vol. A47, p. 110, 1991), the graphical display program GRASP, or the graphical display program INSIGHT. Suitable computer hardware useful for producing an image of the present invention are known to those of skill in the art (e.g., a Silicon Graphics Workstation).

A representation, or model, of the three dimensional structure of the CR2-C3d complex structure for which a crystal has been produced can also be determined using techniques which include molecular replacement or SIR/MIR (single/multiple isomorphous replacement). Methods of molecular replacement are generally known by those of skill in the art (generally described in Brunger, *Meth. Enzym.*, vol. 276, pp. 558-580, 1997; Navaza

and Saludjian, *Meth. Enzym.*, vol. 276, pp. 581-594, 1997; Tong and Rossmann, *Meth. Enzym.*, vol. 276, pp. 594-611, 1997; and Bentley, *Meth. Enzym.*, vol. 276, pp. 611-619, 1997, each of which are incorporated by this reference herein in their entirety) and are performed in a software program including, for example, AmoRe (CCP4, *Acta Cryst.* D50, 760-763 (1994) or XPLOR. Briefly, X-ray diffraction data is collected from the crystal of a crystallized target structure. The X-ray diffraction data is transformed to calculate a Patterson function. The Patterson function of the crystallized target structure is compared with a Patterson function calculated from a known structure (referred to herein as a search structure). The Patterson function of the crystallized target structure is rotated on the search structure Patterson function to determine the correct orientation of the crystallized target structure in the crystal. The translation function is then calculated to determine the location of the target structure with respect to the crystal axes. Once the crystallized target structure has been correctly positioned in the unit cell, initial phases for the experimental data can be calculated. These phases are necessary for calculation of an electron density map from which structural differences can be observed and for refinement of the structure. Preferably, the structural features (e.g., amino acid sequence, conserved di-sulphide bonds, and β-strands or β-sheets) of the search molecule are related to the crystallized target structure.

As used herein, the term "model" refers to a representation in a tangible medium of the three dimensional structure of a protein, polypeptide or peptide. For example, a model can be a representation of the three dimensional structure in an electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. The

phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Hard copies include both motion and still pictures. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α carbon traces, ribbon diagrams and electron density maps.

Preferably, a three dimensional structure of a CR2 protein provided by the present invention includes: (a) a structure defined by atomic coordinates of a three dimensional structure of a crystalline CR2 SCR1-2 region in complex with C3d; (b) a structure defined by atomic coordinates selected from the group consisting of: (i) atomic coordinates represented in a table selected from the group consisting of Table 2 (CR2-C3d) and Table 3 (CR2 only); and, (ii) atomic coordinates that define a three dimensional structure, wherein at least 50% of the structure has an average root-mean-square deviation (RMSD) from backbone atoms in secondary structure elements in at least one domain of a three dimensional structure represented by the atomic coordinates of (1) of equal to or less than about 1.0Å; and/or (c) a structure defined by atomic coordinates derived from CR2 protein molecules arranged in a crystalline manner in a space group R3 or R32 so as to form a unit cell of dimensions a=b=170.5A, c=173.8 A.

The present inventors have provided the atomic coordinates that define the three dimensional structure of a crystalline CR2 short consensus repeat (SCR) 1-2 region (CR2 SCR1-2 region) in complex with C3d. Using the guidance provided herein, one of skill in the art will be able to reproduce such a crystalline structure and define atomic coordinates of such a structure. Example 1 demonstrates the production of a CR2-C3d complex (CR2 SCR1-2 region in complex with C3d) arranged in a crystalline manner in a space group R3 or R32 so as to form a unit cell of dimensions a=b=170.5Å, c=173.8 Å. The atomic coordinates determined from this crystal structure are represented in Table 2. Additionally, these atomic coordinates were deposited on January 11, 2001, with the Protein Data Bank (PDB), operated by the Research Collaboratory for Structural Bioinformatics (RCSB) (H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov,

P.E.Bourne, The Protein Data Bank; *Nucleic Acids Research*, 28:235-242 (2000)), under PDB Deposit No. PDB id 1GHQ. The atomic coordinates in Table 3 are the coordinates that define the three dimensional structure of just the CR2 SCR1-SCR2 domains of the CR2-C3d complex (i.e., the coordinates defining the C3d portion have been removed).

In one embodiment, a three dimensional structure of a CR2 protein provided by the present invention includes a structure represented by atomic coordinates that define a three dimensional structure, wherein at least 50% of the structure has an average root-mean-square deviation (RMSD) from backbone atoms in secondary structure elements in at least one domain of a three dimensional structure represented by the atomic coordinates of Table 2 or Table 3 of equal to or less than about 1.0Å. Such a structure can be referred to as a structural homologue of the CR2 structures defined by Tables 2 and 3. Preferably, at least 50% of the structure has an average root-mean-square deviation (RMSD) from backbone atoms in secondary structure elements in at least one domain of a three dimensional structure represented by the atomic coordinates of Table 2 or Table 3 of equal to or less than about 0.7 Å, equal to or less than about 0.5 Å, and most preferably, equal to or less than about 0.3 Å. In a more preferred embodiment, a three dimensional structure of a CR2 protein provided by the present invention includes a structure defined by atomic coordinates that define a three dimensional structure, wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average root-mean-square deviation (RMSD) value, and most preferably, about 100% of such structure has the recited average root-mean-square deviation (RMSD) value.

In one embodiment, RMSD of a structural homologue of CR2 can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structural homologue and to the structure that is actually represented by such atomic coordinates. Preferably, at least 50% of the structure has an average root-mean-square deviation (RMSD)

from common amino acid side chains in at least one domain of a three dimensional structure represented by the atomic coordinates of Table 2 or Table 3 of equal to or less than about 1.0Å equal to or less than about 0.7 Å, equal to or less than about 0.5 Å, and most preferably, equal to or less than about 0.3 Å. In a more preferred embodiment, a three dimensional structure of a CR2 protein provided by the present invention includes a structure defined by atomic coordinates that define a three dimensional structure, wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average root-mean-square deviation (RMSD) value, and most preferably, about 100% of such structure has the recited average root-mean-square deviation (RMSD) value.

One embodiment of the present invention relates to a method of structure-based identification of compounds which potentially bind to complement receptor type 2 (CR2) proteins or to a complex of CR2 and its ligand, comprising: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region; and (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region. The three dimensional structure of the CR2 SCR 1-2 region is selected from the group of:

(i) a structure defined by atomic coordinates of a three dimensional structure of a crystalline CR2 SCR1-2 region in complex with C3d;

(ii) a structure defined by atomic coordinates selected from the group consisting of:

(1) atomic coordinates represented in a table selected from the group consisting of Table 2 (CR2-C3d) and Table 3 (CR2 only);

(2) atomic coordinates that define a three dimensional structure, wherein at least 50% of the structure has an average root-mean-square deviation (RMSD) from backbone atoms in secondary structure elements in at least one

domain of a three dimensional structure represented by the atomic coordinates of (1) of equal to or less than about 1.0Å; and

(iii) a structure defined by atomic coordinates derived from CR2 protein molecules arranged in a crystalline manner in a space group R3 or R32 so as to form a unit cell of dimensions a=b=170.5Å, c=173.8 Å.

The structures used to perform the above-described method have been described in detail above and in the Examples section. According to the present invention, the phrase "providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region" is defined as any means of providing, supplying, accessing, displaying, retrieving, or otherwise making available the three dimensional structure of the CR2 short consensus repeat (SCR) 1-2 region described herein. For example, the step of providing can include, but is not limited to, accessing the atomic coordinates for the structure from a database; importing the atomic coordinates for the structure into a computer or other database; displaying the atomic coordinates and/or a model of the structure in any manner, such as on a computer, on paper, etc.; and determining the three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region *de novo* using the guidance provided herein.

The second step of the method of structure based identification of compounds of the present invention includes identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region. CR2 is a receptor for at least three biologically important ligands, and has been shown to play a role in several aspects of the humoral immune response, EBV infection, and HIV-1 infection. Therefore, identification and/or design of compounds that mimic, enhance, disrupt or compete with the interactions of CR2 with its ligands are highly desirable. Such compounds can be designed using structure based drug design. Until the discovery of the three dimensional structure of the present invention, the only information available for the development of therapeutic compounds based on the CR2 protein was based on the primary

sequence of the CR2 protein. Structure based drug design refers to the prediction of a conformation of a peptide, polypeptide, protein, or conformational interaction between a peptide or polypeptide, and a compound, using the three dimensional structure of the peptide, polypeptide or protein. Typically, structure based drug design is performed with a computer. For example, generally, for a protein to effectively interact with (e.g., bind to) a compound, it is necessary that the three dimensional structure of the compound assume a compatible conformation that allows the compound to bind to the protein in such a manner that a desired result is obtained upon binding. Knowledge of the three dimensional structure of the protein enables a skilled artisan to design a compound having such compatible conformation, or to select such a compound from available libraries of compounds. For example, knowledge of the three dimensional structure of the C3d binding site of CR2 enables one of skill in the art to design a compound that binds to CR2, is stable and results in, for example, inhibition of a biological response such as C3d binding to CR2, or cellular signal transduction through the CR2, upon such binding. In addition, for example, knowledge of the three dimensional structure of the C3d binding site of a CR2 enables a skilled artisan to design a substrate analog of CR2.

Suitable structures and models useful for structure based drug design are disclosed herein. Preferred target structures to use in a method of structure based drug design include any representations of structures produced by any modeling method disclosed herein, including molecular replacement and fold recognition related methods.

According to the present invention, the step of designing a compound for testing in a method of structure based identification of the present invention can include creating a new chemical compound or searching databases of libraries of known compounds (e.g., a compound listed in a computational screening database containing three dimensional structures of known compounds). Designing can also be performed by simulating chemical compounds having substitute moieties at certain structural features. The step of designing can include selecting a chemical compound based on a known function of the compound.

A preferred step of designing comprises computational screening of one or more databases of compounds in which the three dimensional structure of the compound is known and is interacted (e.g., docked, aligned, matched, interfaced) with the three dimensional structure of a CR2 by computer (e.g. as described by Humblet and Dunbar, *Animal Reports in Medicinal Chemistry*, vol. 28, pp. 275-283, 1993, M Venuti, ed., Academic Press). Methods to synthesize suitable chemical compounds are known to those of skill in the art and depend upon the structure of the chemical being synthesized. Methods to evaluate the bioactivity of the synthesized compound depend upon the bioactivity of the compound (e.g., inhibitory or stimulatory) and are disclosed herein.

Various other methods of structure-based drug design are disclosed in Maulik et al., 1997, *Molecular Biotechnology: Therapeutic Applications and Strategies*, Wiley-Liss, Inc., which is incorporated herein by reference in its entirety. Maulik et al. disclose, for example, methods of directed design, in which the user directs the process of creating novel molecules from a fragment library of appropriately selected fragments; random design, in which the user uses a genetic or other algorithm to randomly mutate fragments and their combinations while simultaneously applying a selection criterion to evaluate the fitness of candidate ligands; and a grid-based approach in which the user calculates the interaction energy between three dimensional receptor structures and small fragment probes, followed by linking together of favorable probe sites.

In a molecular diversity strategy, large compound libraries are synthesized, for example, from peptides, oligonucleotides, carbohydrates and/or synthetic organic molecules, using biological, enzymatic and/or chemical approaches. The critical parameters in developing a molecular diversity strategy include subunit diversity, molecular size, and library diversity. The general goal of screening such libraries is to utilize sequential application of combinatorial selection to obtain high-affinity ligands for a desired target, and then to optimize the lead molecules by either random or directed design strategies. Methods of molecular diversity are described in detail in Maulik, et al., ibid.

Maulik et al. also disclose, for example, methods of directed design, in which the user directs the process of creating novel molecules from a fragment library of appropriately selected fragments; random design, in which the user uses a genetic or other algorithm to randomly mutate fragments and their combinations while simultaneously applying a selection criterion to evaluate the fitness of candidate ligands; and a grid-based approach in which the user calculates the interaction energy between three dimensional receptor structures and small fragment probes, followed by linking together of favorable probe sites.

In the present method of structure based drug design, it is not necessary to align a candidate chemical compound (i.e., a chemical compound being analyzed in, for example, a computational screening method of the present invention) to each residue in a target site (target sites will be discussed in detail below). Suitable candidate chemical compounds can align to a subset of residues described for a target site. Preferably, a candidate chemical compound comprises a conformation that promotes the formation of covalent or noncovalent crosslinking between the target site and the candidate chemical compound. Preferably, a candidate chemical compound binds to a surface adjacent to a target site to provide an additional site of interaction in a complex. When designing an antagonist (i.e., a chemical compound that inhibits the binding of a ligand to CR2 by blocking a binding site or interface), for example, the antagonist should bind with sufficient affinity to the binding site or to substantially prohibit a ligand (i.e., a molecule that specifically binds to the target site) from binding to a target area. It will be appreciated by one of skill in the art that it is not necessary that the complementarity between a candidate chemical compound and a target site extend over all residues specified here in order to inhibit or promote binding of a ligand.

In general, the design of a chemical compound possessing stereochemical complementarity can be accomplished by techniques that optimize, chemically or geometrically, the "fit" between a chemical compound and a target site. Such techniques are disclosed by, for example, Sheridan and Venkataraghavan, *Acc. Chem Res.*, vol. 20, p. 322, 1987; Goodford, *J. Med. Chem.*, vol. 27, p. 557, 1984; Beddell, *Chem. Soc. Reviews*, vol.

279, 1985; Hol, *Angew. Chem.*, vol. 25, p. 767, 1986; and Verlinde and Hol, *Structure*, vol. 2, p. 577, 1994, each of which are incorporated by this reference herein in their entirety.

One embodiment of the present invention for structure based drug design comprises identifying a chemical compound that complements the shape of a CR2, including a portion of CR2, such as the SCR1-SCR2 region. Such method is referred to herein as a "geometric approach". In a geometric approach, the number of internal degrees of freedom (and the corresponding local minima in the molecular conformation space) is reduced by considering only the geometric (hard-sphere) interactions of two rigid bodies, where one body (the active site) contains "pockets" or "grooves" that form binding sites for the second body (the complementing molecule, such as a ligand).

The geometric approach is described by Kuntz et al., *J. Mol. Biol.*, vol. 161, p. 269, 1982, which is incorporated by this reference herein in its entirety. The algorithm for chemical compound design can be implemented using the software program DOCK Package, Version 1.0 (available from the Regents of the University of California). Pursuant to the Kuntz algorithm, the shape of the cavity or groove on the surface of a structure (e.g., CR2) at a binding site or interface is defined as a series of overlapping spheres of different radii. One or more extant databases of crystallographic data (e.g., the Cambridge Structural Database System maintained by University Chemical Laboratory, Cambridge University, Lensfield Road, Cambridge CB2 1EW, U.K.) or the Protein Data Bank maintained by Brookhaven National Laboratory, is then searched for chemical compounds that approximate the shape thus defined.

Chemical compounds identified by the geometric approach can be modified to satisfy criteria associated with chemical complementarity, such as hydrogen bonding, ionic interactions or Van der Waals interactions.

Another embodiment of the present invention for structure based identification of compounds comprises determining the interaction of chemical groups ("probes") with an active site at sample positions within and around a binding site or interface, resulting in an

array of energy values from which three dimensional contour surfaces at selected energy levels can be generated. This method is referred to herein as a "chemical-probe approach." The chemical-probe approach to the design of a chemical compound of the present invention is described by, for example, Goodford, *J. Med. Chem.*, vol. 28, p. 849, 1985, which is incorporated by this reference herein in its entirety, and is implemented using an appropriate software package, including for example, GRID (available from Molecular Discovery Ltd., Oxford OX2 9LL, U.K.). The chemical prerequisites for a site-complementing molecule can be identified at the outset, by probing the active site of a CR2, for example, (as represented by the atomic coordinates shown in Table 2 or Table 3) with different chemical probes, e.g., water, a methyl group, an amine nitrogen, a carboxyl oxygen and/or a hydroxyl. Preferred sites for interaction between an active site and a probe are determined. Putative complementary chemical compounds can be generated using the resulting three dimensional pattern of such sites.

According to the present invention, suitable candidate compounds to test using the method of the present invention include proteins, peptides or other organic molecules, and inorganic molecules. Suitable organic molecules include small organic molecules. Peptides refer to small molecular weight compounds yielding two or more amino acids upon hydrolysis. A polypeptide is comprised of two or more peptides. As used herein, a protein is comprised of one or more polypeptides. Preferred therapeutic compounds to design include peptides composed of "L" and/or "D" amino acids that are configured as normal or retroinverso peptides, peptidomimetic compounds, small organic molecules, or homo- or hetero-polymers thereof, in linear or branched configurations.

Preferably, a compound that is identified by the method of the present invention originates from a compound having chemical and/or stereochemical complementarity with CR2 and/or C3d. Such complementarity is characteristic of a compound that matches the surface of the receptor either in shape or in distribution of chemical groups and binds to CR2 to promote or inhibit CR2 ligand binding, or to induce cellular signal transduction in a cell

expressing CR2 upon the binding of the compound to CR2. More preferably, a compound that binds to a ligand binding site of CR2 associates with an affinity of at least about 10^{-6} M, and more preferably with an affinity of at least about 10^{-7}M, and more preferably with an affinity of at least about 10^{-8} M.

Preferably, three general sites of the CR2 are targets for structure based drug design (i.e., target sites), although other sites may become apparent to those of skill in the art. The three preferred sites include: (1) the interface between CR2 and C3d; (2) the interface between the SCR1 and SCR2 domains of CR2; and (3) the dimerization interface between two CR2 monomers. Combinations of any of these general sites are also suitable target sites. The interface between CR2 and C3d is depicted in Fig. 1A, and Figs. 3A-3E. The interface between the SCR1 and SCR2 domains of CR2 is depicted in Figs. 2A-2C. The dimer interface between CR2 monomeric proteins is depicted in Figs. 1B, 2D and 6A. The following discussion provides specific detail on compound identification (e.g., drug design) using target sites of the CR2 based on its three-dimensional structure in complex with C3d. It is to be understood, however, that one of skill in the art, using the description of the CR2 structure provided herein, will be able to identify compounds that are potential candidates for inhibiting, stimulating or enhancing the interaction of CR2 with its other ligands.

The C3d binding site (i.e., the interface between CR2 and C3d) is targeted to directly affect the binding of CR2 to C3d, other CR2-binding C3 fragments, or another ligand (i.e., inhibition or enhancement). In the CR2-C3d complex, no continuous stretch of residues on C3d participates in the interactions. Rather, residues that are separated in the linear sequence of C3d, but come together on the folded C3d, interact with CR2. Namely, the residues on the H3-H4 loop (the loop between helix 3 and 4), as well as H5, and H7 make contact with CR2 (Fig. 3C). On the CR2 part, however, a linear stretch of residues within SCR2 domain makes the contact with C3d. The B strand and B-C loop of SCR2 constitute the majority of the interactions with C3d. The nature of the contacts involves elegant networks of hydrogen bonds, plus some hydrophobic and van der Waals interactions (Fig. 3D & 3E). The contact

site is discussed in detail in the Examples. Preferred target sites in the C3d binding interface with CR2 include, but are not limited to: (1) a site on the B strand and the B-C loop of CR2 SCR2 comprising the segment: G79-G80-Y81-K82-I83-R84-G85-S86-T87-P88-Y89; (2) a site on the B strand of CR2 SCR2 comprising position K100; (3) a segment of CR2 SCR2 comprising V130-F131-P132-L133; and (4) a segment of CR2 SCR2 comprising the fragment T101-N102-F103. In the T101-N102-F103 site, the N102 residue is glycosylated. The N-acetylglucosamine residue attached to N102 forms a hydrogen bond with C3d. The present inventors have shown that amino acid residues at positions 84 and 86 of SEQ ID NO:4 are particularly important residues in the binding of C3d to CR2 and therefore, segments of CR2 including these residues are particularly desirable target sites. Alternatively, the CR2 contact points on C3d can be targeted for the identification of compounds that specifically modify the interaction between CR2 and C3d (and potentially the interaction of CR2 with its other ligands). Such sites include, but are not limited to: (1) the loop between helix 2-3 of C3d comprising the segment Q68-P69-S70-S71; (2) Helix 5 of C3d comprising the segment S104-Q105-V106-L107-C108-G109-A110-V111-K112-W113-L114-I115-L116-E117-K118-Q119-K120-P121-D122; and (3) Helix 7of C3d comprising the segment N170-S171-L172-P173-G174-S175-I176-T177-K178-A179-G180-D181-F182-L183-E184-A185 (all positions are given with respect to SEQ ID NO:7).

The interface between the two monomers of CR2 can also be targeted to affect the binding of CR2 to a ligand. Two CR2 molecules dimerize through SCR1-SCR1 contacts in the crystal structure (Fig. 2D). The contact is symmetrical, with the E1 strands from different molecules running anti-parallel to each other. The C-terminus of the E1 strand also contacts the C-terminus of the D2 strand of another molecule. The nature of the interaction is hydrogen bonds. Without being bound by theory, the present inventors believe that a CR2 dimer, in contrast to a monomer, can allow a dramatic increase of cross-linked CR2/CD19/CD81 and B cell receptor molecules through binding to the antigen with two or more C3d attached, which can cause a 10,000-fold enhancement of the humoral immune

response. Therefore, compounds that disrupt the dimer formation are expected to be primarily inhibitory compounds with regard to immune responses. Such compounds may also be beneficial, however, in inhibiting EBV or HIV infection mediated by CR2. Similarly, compounds that enhance or stabilize the dimer formation are expected to stimulate or enhance an immune response.

The interface between the SCR1 and SCR2 domains of CR2 is also targeted to affect the binding of CR2 to a ligand (i.e., inhibit or enhance). The packing of the two SCR domains in CR2 forms a V shape. Residues important for the tight packing between the two domains at the interface and the linker regions are shown in Fig. 2B. A very unique feature of the two domain CR2 structure is that the 8 amino acid linker makes a dramatic turn to allow the two SCR domains to pack against each other sideways (Figs. 2A, 2B, 2C). Among the protein family containing SCR domains, the linkers connecting SCR domains are normally 3-5 amino acids in length, while an 8 amino acid linker is the longest known so far. The available structures of four SCR proteins containing two or 4 repeats (A. P. Wiles, et al.,(1997), *supra*; P. N. Barlow, et al., (1993), *supra*; J. M. Casasnovas, et al.,(1999), *supra*; R. Schwarzenbacher et al., (1999), *supra*) all have end-end packing between consecutive SCRs, and CR2 is thus the first to demonstrate extensive side-side packing. In end-end packing, the adjacent domains could, in principle, adopt different rotations and bend angles relative to each other in different environments. Indeed, a commonly held concept is that SCRs are not absolutely fixed relative to each other but rather are allowed some freedom to move about this interface (P. N. Barlow, et al., (1993), *ibid.*; J. M. Casasnovas, et al.,(1999), *ibid.*). However, the side-side packing of the CR2 SCR1 and SCR2 would not give the two domains freedom to adopt different orientations, unless some active process is involved to first separate the two domains. The interface between the two domains is mainly hydrophobic (Fig. 2B). Trp112, which is unique to CR2 SCR2 sequence and located on strand D2, plays a critical role in the packing by interacting with Ile39 and the main-chain from SCR1. Trp112 would be unfavorably exposed to the solvent if the two domains do not

pack against each other sideways in this manner. In addition to Trp112, several other residues also play a role in the packing, including Pro121, His91, Leu39, and the carbon side chain of Glu64. The 8 amino acid linker, which contains mainly hydrophobic residues such as Tyr65, Phe66, Tyr69, also participates in the hydrophobic packing outside the two-domain interface, further solidifying the interactions between SCR1 and SCR2 (Fig. 2B). The area of the interface of the two SCRs is very extensive, covering almost half of the length of one SCR domain (Fig. 2C). Since the above-mentioned previous studies of other SCR proteins were performed in the absence of their ligands, it is possible that this interface may change upon binding of CR2 to its ligand. In any event, it is predicted that the binding of a compound to this site will have an effect on the ligand-binding ability of CR2.

A candidate compound for binding to a CR2 protein, including to one of the preferred target sites described above, is identified by one or more of the methods of structure-based identification discussed above. As used herein, a "candidate compound" refers to a compound that is selected by a method of structure-based identification described herein as having a potential for binding to a CR2 protein (or its ligand) on the basis of a predicted conformational interaction between the candidate compound and the target site of the CR2 protein. The ability of the candidate compound to actually bind to a CR2 protein can be determined using techniques known in the art, as discussed in some detail below. A "putative compound" is a compound with an unknown regulatory activity, at least with respect to the ability of such a compound to bind to and/or regulate CR2 as described herein. Therefore, a library of putative compounds can be screened using structure based identification methods as discussed herein, and from the putative compounds, one or more candidate compounds for binding to CR2 can be identified. Alternatively, a candidate compound for binding to CR2 can be designed *de novo* using structure based drug design, also as discussed above. Candidate compounds can be selected based on their predicted ability to inhibit the binding of CR2 to its ligand, to stabilize (e.g., enhance) the binding of CR2 to its ligand, to bind to and activate CR2, to bind to and inhibit the activation of CR2,

to bind to and activate a ligand of CR2, to bind to and inhibit the activation of a ligand of CR2, to disrupt the dimerization of CR2 monomers, or to stabilize the dimerization of CR2 monomers.

Accordingly, in one aspect of the present invention, the method of structure-based identification of compounds that potentially bind to complement receptor type 2 (CR2) proteins or to a complex of CR2 and its ligand further includes steps which confirm whether or not a candidate compound has the predicted properties with respect to its effect on CR2 (or a ligand of CR2). In one embodiment, the candidate compound is predicted to be an inhibitor of the binding of CR2 to its ligand, and the method further includes: (c) contacting the candidate compound identified in step (b) with CR2 or a fragment thereof and a CR2 ligand or a fragment thereof under conditions in which a CR2-CR2 ligand complex can form in the absence of the candidate compound; and (d) measuring the binding affinity of the CR2 or fragment thereof to the CR2 ligand or fragment thereof. A candidate inhibitor compound is selected as a compound that inhibits the binding of CR2 to its ligand when there is a decrease in the binding affinity of the CR2 or fragment thereof for the CR2 ligand or fragment thereof, as compared to in the absence of the candidate inhibitor compound.

In another embodiment, the candidate compound is predicted to be a stabilizer of the binding of CR2 to its ligand, and the method further comprises: (c) contacting the candidate compound identified in step (b) with a CR2-CR2 ligand complex, wherein the CR2-CR2 ligand complex comprises CR2 or a fragment thereof and a CR2 ligand, or a fragment thereof; (d) measuring the stability of the CR2-CR2 ligand complex of (i). A candidate stabilizer compound is selected as a compound that stabilizes the CR2-CR2 ligand complex when there is an increase in the stability of the complex as compared to in the absence of the candidate stabilizer compound.

In another embodiment, the candidate compound is predicted to bind to and activate CR2 (i.e., an agonist), and the method further comprises: (c) contacting the candidate compound identified in step (b) with CR2 or a ligand-binding fragment thereof, under

conditions wherein in the absence of the compound, CR2 is not activated; and, (d) measuring the ability of the candidate compound to bind to CR2 to activate CR2. A candidate agonist compound is selected as a compound that binds to CR2 and activates CR2 as compared to in the absence of the candidate agonist compound. A similar embodiment includes the identification of candidate compounds that bind to target sites on the CR2 ligand which are now known as a result of the present inventors' work, and the determination of the ability of the candidate compound to bind to and activate the ligand of CR2 (e.g., by mimicking the structure of CR2).

In another embodiment, the candidate compound is predicted to bind to and inhibit CR2 (i.e., an antagonist), and the method further comprises: (c) contacting the candidate compound identified in step (b) with CR2 or a ligand-binding fragment thereof, wherein in the absence of the compound, CR2 is not activated; and, (d) measuring the ability of the candidate compound to bind to CR2 and activate CR2. A candidate antagonist compound is selected as a compound that binds to CR2 but does not activate and, in some embodiments, inhibits any constitutive activation, of the CR2. A similar embodiment includes the identification of candidate compounds that bind to target sites on the CR2 ligand which are now known as a result of the present inventors' work, and the determination of the ability of the candidate compound to bind to but not activate the ligand of CR2.

In another embodiment, the candidate compound is predicted to bind to CR2 and to disrupt the dimerization of CR2 monomers, and the method further comprises: (c) contacting the candidate compound identified in step (b) with at least two CR2 monomers or ligand-binding fragments thereof, in the presence and in the absence of a CR2 ligand or fragment thereof; and, (d) measuring the ability of the candidate compound to bind to CR2, the ability of the CR2 monomers to dimerize, and/or the ability of the CR2 ligand to activate CR2. A candidate compound for the disruption of CR2 dimerization is selected as a compound that binds to CR2 but inhibits the dimerization of CR2 and in some embodiments, inhibits the activation of CR2 by its ligand. Similarly, a candidate compound for stabilizing the

dimerization of CR2 is a compound that binds to CR2, prolongs the dimerization of CR2 as compared to in the absence of the candidate compound, and in some embodiments, enhances or prolongs the activation of CR2 by its ligand.

In one embodiment, the conditions under which a CR2 according to the present invention is contacted with a candidate compound, such as by mixing, are conditions in which the receptor is not stimulated (activated) or bound to a natural ligand if essentially no candidate compound is present. For example, such conditions include normal culture conditions in the absence of a stimulatory compound (a stimulatory compound being, e.g., the natural ligand for the receptor (e.g., C3d, CD23, EBV), a stimulatory antibody, or other equivalent stimulus). In this embodiment, the candidate compound is then contacted with the CR2. In this embodiment, the step of detecting is designed to indicate whether the candidate compound binds to CR2, and in some embodiments, whether the candidate compound activates CR2.

In an alternate embodiment, the conditions under which a CR2 according to the present invention is contacted with a candidate compound, such as by mixing, are conditions in which the receptor is normally bound by a ligand or additionally stimulated (activated) if essentially no candidate compound is present. Such conditions can include, for example, contact of CR2 with a stimulator molecule (a stimulatory compound being, e.g., the natural ligand for the receptor, a stimulatory antibody, or other equivalent stimulus) which binds to the receptor and causes the receptor to become activated. In this embodiment, the candidate compound can be contacted with the receptor prior to the contact of the receptor with the stimulatory compound (e.g., to determine whether the candidate compound blocks or otherwise inhibits the binding and/or stimulation of CR2 by the stimulatory compound), or after contact of the receptor with the stimulatory compound (e.g., to determine whether the candidate compound downregulates, or reduces the activation of the receptor).

The present methods involve contacting CR2 with the candidate compound being tested for a sufficient time to allow for binding to, activation or inhibition of the receptor by

the candidate compound. The period of contact with the candidate compound being tested can be varied depending on the result being measured, and can be determined by one of skill in the art. For example, for binding assays, a shorter time of contact with the candidate compound being tested is typically suitable, than when activation is assessed. As used herein, the term "contact period" refers to the time period during which the CR2 molecules are in contact with the compound being tested. The term "incubation period" refers to the entire time during which cells expressing CR2, for example, are allowed to grow prior to evaluation, and can be inclusive of the contact period. Thus, the incubation period includes all of the contact period and may include a further time period during which the compound being tested is not present but during which growth is continuing (in the case of a cell based assay) prior to scoring. The incubation time for growth of cells can vary but is sufficient to allow for the binding of CR2, activation of the receptor or signal transduction pathways associated with the receptor, and/or inhibition of the receptor. It will be recognized that shorter incubation times are preferable because compounds can be more rapidly screened. A preferred incubation time is between about 1 minute to about 48 hours.

In accordance with the present invention, a cell-based assay is conducted under conditions which are effective to screen for candidate compounds useful in the method of the present invention. Effective conditions include, but are not limited to, appropriate media, temperature, pH and oxygen conditions that permit the growth of the cell that expresses the receptor. An appropriate, or effective, medium refers to any medium in which a cell that naturally or recombinantly expresses a CR2, when cultured, is capable of cell growth and expression of CR2. Such a medium is typically a solid or liquid medium comprising growth factors and assimilable carbon, nitrogen and phosphate sources, as well as appropriate salts, minerals, metals and other nutrients, such as vitamins. Culturing is carried out at a temperature, pH and oxygen content appropriate for the cell. Such culturing conditions are within the expertise of one of ordinary skill in the art.

Cells that are useful in the cell-based assays of the present invention include any cell that expresses a CR2 and particularly, other proteins that are associated with CR2 signal transduction cascades (e.g., the CR2/CD19/CD81 co-activation complex (D. T. Fearon, 1995 *ibid.*; D. T. Fearon, 1998, *ibid.*; J. C. Cambier, 1997, *ibid.*; A. K. Matsumoto, et al., *J Exp Med* 173, 55-64 (1991))). Such cells include B lymphocytes, T lymphocytes, follicular dendritic cells, thymocytes, epithelial cells, and mast cells. Additionally, certain cells may be induced to express CR2, for example, some tumor cells. Therefore, cells that express CR2 can include cells that naturally express CR2, recombinantly express CR2, or which can be induced to express CR2. Cells useful in some embodiments can also include cells that express a natural ligand of CR2, such as CD23.

The assay of the present invention can also be a non-cell based assay. In this embodiment, the candidate compound can be directly contacted with an isolated CR2, or a receptor component (e.g., an isolated extracellular portion of the receptor, or soluble receptor), and the ability of the candidate compound to bind to the receptor or receptor component can be evaluated, such as by an immunoassay or other binding assay. The assay can, if desired, additionally include the step of further analyzing whether candidate compounds which bind to a portion of the receptor are capable of increasing or decreasing the activity of CR2. Such further steps can be performed by cell-based assay, as described above, or by non-cell-based assay. For example, isolated membranes may be used to identify compounds that interact with CR2. Membranes can be harvested from cells expressing CR2 by standard techniques and used in an *in vitro* binding assay. ^{125}I-labeled (other labels can be used also) ligand (*e.g.*, ^{125}I-labeled C3d) is contacted with the membranes and assayed for specific activity; specific binding is determined by comparison with binding assays performed in the presence of excess unlabeled ligand. Membranes are typically incubated with labeled ligand in the presence or absence of test compound. Compounds that bind to the receptor and compete with labeled ligand for binding to the membranes reduced the signal compared to the vehicle control samples.

Alternatively, soluble CR2 may be recombinantly expressed and utilized in non-cell based assays to identify compounds that bind to CR2. Recombinantly expressed CR2 polypeptides or fusion proteins containing one or more extracellular domains of CR2, and preferably, at least SCR1 and SCR2, can be used in the non-cell based screening assays. Alternatively, peptides corresponding to the extracellular domain of CR2 or fusion proteins containing the extracellular domain of CR2 can be used in non-cell based assay systems to identify compounds that bind to the extracellular portion of CR2. In non-cell based assays the recombinantly expressed CR2 is attached to a solid substrate by means well known to those in the art. For example, CR2 and/or cell lysates containing such receptors can be immobilized on a substrate such as: artificial membranes, organic supports, biopolymer supports and inorganic supports. The protein can be immobilized on the solid support by a variety of methods including adsorption, cross-linking (including covalent bonding), and entrapment. Adsorption can be through van del Waal's forces, hydrogen bonding, ionic bonding, or hydrophobic binding. Exemplary solid supports for adsorption immobilization include polymeric adsorbents and ion-exchange resins. Solid supports can be in any suitable form, including in a bead form, plate form, or well form. The test compounds are then assayed for their ability to bind to CR2.

In one embodiment, a BIAcore machine can be used to determine the binding constant of a complex between CR2 and a ligand (e.g., C3d) in the presence and absence of the candidate compound. For example, CR2 or a ligand binding fragment thereof can be immobilized on a substrate. A ligand, such as C3d, is contacted with the substrate to form a CR2-C3d complex. The dissociation constant for the complex can be determined by monitoring changes in the refractive index with respect to time as buffer is passed over the chip (O'Shannessy et al. Anal. Biochem. 212:457-468 (1993); Schuster et al., Nature 365:343-347 (1993)). Contacting a candidate compound at various concentrations with the CR2-ligand complex and monitoring the response function (e.g., the change in the refractive index with respect to time) allows the complex dissociation constant to be determined in the

presence of the candidate compound and indicates whether the candidate compound is either an inhibitor or an agonist of the CR2-ligand complex. Alternatively, the candidate compound can be contacted with the immobilized CR2 at the same time as the ligand to see if the candidate compound inhibits or stabilizes the binding of the ligand to CR2.

Other suitable assays for measuring the binding of a candidate compound to a CR2 or CR2 ligand, and or for measuring the ability of such compound to affect the binding of a CR2 to its ligand include, for example, immunoassays such as enzyme linked immunoabsorbent assays (ELISA) and radioimmunoassays (RIA), as well as cell-based assays including, cytokine secretion assays, or intracellular signal transduction assays that determine, for example, protein or lipid phosphorylation, mediator release or intracellular Ca^{++} mobilization upon CR2 binding to a cell signal transduction molecule or coreceptor.

As used herein, the phrase "agonist" refers to any compound that interacts with a CR2 and elicits an observable response. More particularly, a CR2 agonist can include, but is not limited to, a protein (including an antibody), a peptide, a nucleic acid or any suitable product of drug design (e.g., a mimetic) which is characterized by its ability to agonize (e.g., stimulate, induce, increase, enhance) the biological activity of a naturally occurring CR2 in a manner similar to a natural agonist (e.g., C3d, gp350/220, or CD23) (e.g., by interaction/binding with and/or direct or indirect activation of CR2, including by stabilizing the interaction of CR2 with a natural ligand). An "antagonist" refers to any compound which inhibits the effect of a CR2 agonist, as described above. More particularly, a CR2 antagonist is capable of associating with a CR2 such that the biological activity of the receptor is decreased (e.g., reduced, inhibited, blocked, reversed, altered) in a manner that is antagonistic (e.g., against, a reversal of, contrary to) to the action of a natural agonist on the receptor. It is noted that the three dimensional structures disclosed herein can be used to design or identify candidate compounds that agonize or antagonize the biological activity of the CR2 ligand. For example, a compound that enhances the interaction between CR2 and CD23 can also have a stimulatory effect on a cell that expresses CD23.

Preferred agonists (i.e., stimulatory compounds) to identify using the present method are compounds that exhibit improved binding to CR2 when compared with the ability of a natural CR2 ligand to bind to CR2, and also include compounds that enhance the binding of a natural ligand to CR2 or enhance signal transduction through CR2 coreceptor complexes. Preferred agonists of the present invention are identified by their ability to: (1) bind to, or otherwise interact with, CR2 at a higher level than, for example, a natural CR2 ligand; (2) enhance binding of CR2 to its ligand; (3) enhance dimer formation of CR2 by binding to CR2 or to the combination of CR2 bound to its ligand; and/or (4) enhance signal transduction through CR2. A preferred agonist of the present invention can also include a compound that binds to CR2 or a CR2 ligand, thereby enhancing the binding of CR2 to its ligand or improving cellular signal transduction during or after the binding of CR2 to its ligand, by, for example, modifying other regions of the CR2 by an allosteric interaction that modifies the ligand-binding site of CR2. Another suitable agonist compound of the present invention can include a compound that binds to CR2 in the absence of a natural ligand, in such a manner that CR2-mediated cellular signal transduction is stimulated.

Suitable antagonist (i.e., inhibitory) compounds to identify using the present method are compounds that interact directly with CR2, thereby inhibiting the binding of a natural ligand to CR2, by either blocking the ligand binding site of CR2 (referred to herein as substrate analogs) or by modifying other regions of CR2 (such as in the interface between the monomers of a CR2 dimer, or at the interface between the SCR1 and SCR2 regions of each monomer) such that the natural ligand cannot bind to CR2 (e.g., by allosteric interaction). A CR2 substrate analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the ligand binding site of a CR2 protein. A CR2 substrate analog can, for example, comprise a chemical compound that mimics the CR2 binding portion of a natural ligand, or that binds specifically to the ligand binding site of CR2 but does not mimic the CR2 binding portion of the natural ligand. An inhibitory compound of the present invention can also include a compound that essentially mimics at least a portion of CR2 that

binds to a natural ligand (referred to herein as a peptidomimetic compound). Other suitable inhibitory compounds of the present invention include compounds that inhibit the binding of CR2 to a cell signal inducing molecule such as CD19.

Various specific embodiments of the present invention are described below. The description of the structure of CR2, and of structure based methods of identifying compounds that regulate CR2 are generally applicable to the methods described below, with particular modifications being noted in the specific description of the methods.

One embodiment of the present invention relates to a method to identify a compound that inhibits the complement receptor type 2 (CR2)-dependent infection of a host cell by Epstein Barr Virus (EBV). This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as previously described herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a cell that expresses CR2 or a ligand binding fragment thereof and an Epstein Barr Virus (EBV) particle under conditions in which the EBV particle can bind to CR2 and infect the cell in the absence of the candidate compound; and (d) measuring the intracellular EBV titer of the cell; wherein a candidate inhibitor compound is selected as a compound that inhibits the EBV titer in the cell, as compared to in the absence of the candidate inhibitor compound.

As discussed in the Background section, one of the naturally occurring ligand for human CR2 is Epstein-Barr virus (EBV). EBV interacts with CR2 via the gp350/220 viral membrane protein (J. D. Fingeroth, et al., *Proc Natl Acad Sci U S A* 81, 4510-4 (1984)). EBV causes infectious mononucleosis, and is associated with Burkitt's Lymphoma and several other lymphomas and non-lymphoid tumors (M. Okano, *Acta Paediatr* 87, 11-8 (1998)). Therefore, the identification of compounds that inhibit the interaction between EBV and CR2 are desirable. Previous studies have suggested that two amino acid positions in

CR2 Ser16 and Tyr68 to Tyr, Fig. 2E and green patch in Figs. 5A and 5B) are likely to be involved in gp350/220 binding (D. R. Martin et al., *J Virol* 68, 4716-26 (1994)). Given the three dimensional structure of the CR2 disclosed herein, one of skill in the art can now design or identify compounds that are predicted to bind to three dimensional face of CR2 including these residues.

In this embodiment, the steps of providing the CR2 structure and identifying a candidate compound are performed as described above generally for any candidate compound. The step of contacting the candidate can be performed under any suitable conditions for contacting a virus, or portion of the virus (e.g., gp350/220) with a receptor. Such a method preferably includes contacting (e.g., by mixing, adding, combining) EBV with a cell that expresses CR2 or a ligand binding fragment thereof (e.g., naturally, recombinantly or by induction) under conditions wherein, in the absence of the candidate compound, the EBV particle can bind to CR2 and infect the cell. The intracellular viral titer is measured in the presence and in the absence of the compound using methods well known to those of skill in the art. An inhibitor compound is selected as a compound that inhibits the EBV titer in the cell, as compared to in the absence of the candidate inhibitor compound.

Another embodiment of the present invention relates to a method to identify a compound that inhibits the binding of CD23 to complement receptor type 2 (CR2). This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as previously described herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a first cell expressing CR2 or a ligand binding fragment thereof and a second cell expressing a CD23 protein or fragment thereof under conditions in which the CD23 protein or fragment thereof and the CR2 or the ligand binding fragment thereof can bind in the absence of the candidate compound; and (d) measuring a biological activity

induced by the interaction of CD23 and CR2 in the first or second cell; wherein a candidate inhibitor compound is selected as a compound that inhibits the biological activity as compared to in the absence of the candidate inhibitor compound.

CD23 is a molecule expressed on the follicular dendritic or other cell lineage surfaces which binds to B cells via CR2 (CR2/CD19/CD81 co-activation complex), thereby greatly potentiating signaling via the B cell antigen receptor. The identification of compounds that enhance the binding of CD23 to CR2 would be desirable under conditions when potentiation of the B cell antigen response is desired. However, CD23 is known to enhance IgE isotype switching in B cells. IgE is the prominent immunoglobulin isotype involved in allergic reactions. Inhibition of IgE production would reduce symptoms of allergic inflammation. Therefore, in one embodiment, it is desirable to inhibit the interaction between CR2 and CD23 to reduce IgE isotype switching in B cells.

In this embodiment, the step of contacting the candidate compound identified in step (b) with a first cell expressing CR2 or a ligand binding fragment thereof and a second cell expressing a CD23 protein or fragment thereof occurs under conditions in which the CD23 protein or fragment thereof and the CR2 or the ligand binding fragment thereof can bind in the absence of the candidate compound. Such conditions have been described above for cell-based assays. Preferably, the first cell is a B cell, although any CR2-expressing cell as described herein can be used. The CD23-expressing cell can include a follicular dendritic cell and a cell that recombinantly expresses CD23. Step (d) of measuring a biological activity induced by the interaction of CD23 and CR2 in the first or second cell can include the measurement of any suitable biological activity that is indicative of CR2 activation in the first cell and/or CD23 activation in the second cell. For example, biological activities associated with CR2 activation include, activation of lyn tyrosine kinase, activations of phosphatidyl inositol 3' kinase, phosphorylation of CD19, activation of PI3 kinase, and activation of protein kinase C (PKC). If the CR2-expressing cell is a B cell, isotype switching to IgE can be measured, for example, by comparing the amounts of expression of

IgE between cells in the presence and absence of the compound. Biological activities associated with CD23 activation include, but are not limited to, increases in IgG synthesis, phosphatidylinositol hydrolysis, cAMP synthesis, Calcium flux, protein tyrosine kinase activation, increases in IL-6 and TNF-α synthesis, nitric oxide activation, increases in CD40 and HLA Class II expression, and NF-κB activation (J. Gordon, *Immunol. Today* 15, 411-417 (1994); B. Heyman, *Ann. Rev. Immunol.* 18, 709-737 (2000); V. Fremeaux-Bacchi, et al, *Eur. J. Immunol.* 28, 4268-4274 (1998); R. M. Ten, et al, *J. Immunol.* 163, 3851-3857 (1999). Methods of measuring such biological activities of both CR2 and CD23 are known in the art and include immunoassays, kinase assays, flow cytometry, and phosphorylation assays. In this embodiment of the invention, an inhibitor compound is selected as a compound that inhibits the biological activity of CR2 or CD23 as compared to in the absence of the inhibitor compound.

Yet another embodiment of the present invention relates to a method to identify a compound that inhibits the binding of C3d, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, to complement receptor type 2 (CR2). This method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as previously described herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a cell expressing CR2 or a fragment thereof and C3d or a fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, under conditions in which the C3d or fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, can bind to CR2 and enhance cell activation in the absence of the candidate compound; and (d) measuring the activation of the cell, wherein a candidate inhibitor compound is selected as a compound that inhibits cell activation, as compared to in the absence of the candidate inhibitor compound.

C3d-bound antigens, or antigens containing CR2-binding C3 fragments that contain C3d or a portion thereof, amplify B cell responses by binding to CR2 through C3d (or other CR2-binding C3 fragments that contain C3d or a portion thereof) at the same time as engaging the B cell antigen receptor (BCR) via the bound antigen (R. H. Carter and D. T. Fearon, *Science* 256, 105-7 (1992); J. C. Cambier, *Biochem Soc Trans* 25, 441-5 (1997)). The cross-linking of CR2 to the BCR by C3d greatly amplifies a signal transduction cascade through the CR2/CD19/CD81 co-activation complex (D. T. Fearon, 1995 *ibid.*; D. T. Fearon, 1998, *ibid.*; J. C. Cambier, 1997, *ibid.*; A. K. Matsumoto, et al., *J Exp Med* 173, 55-64 (1991)). Therefore, compounds that inhibit this interaction are useful for reducing an immune response and specifically, a humoral immune response (although effects on the cellular immune response may also be achieved). Compounds that enhance or mimic the interaction between CR2 and C3d are useful for potentiating such an immune response.

In this embodiment, the step of contacting the candidate compound identified in step (b) with a cell expressing CR2 or a fragment thereof and C3d or a fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, occurs under conditions in which the C3d or fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, can bind to CR2 and enhance cell activation in the absence of the candidate compound. Such cell-based methods of contacting have been described previously herein. Preferably, the cell expressing CR2 is selected from the group of a B cell, a T cell, a thymocyte, an epithelial cell, and a mast cell. The measurement of cell activation in (d) can be accomplished by any suitable method for detecting CR2 biological activity as previously described herein, and includes, but is not limited to: the measurement of: cytokine production by the cell, calcium mobilization in the cell, lyn tyrosine kinase activity in the cell, phosphatidyl inositol 3' kinase activity in the cell, phosphorylation of CD19 in the cell, and activation of protein kinase C (PKC) in the cell. An inhibitor compound is selected as a compound that inhibits cell activation, as compared to in the absence of the candidate inhibitor compound.

Another embodiment of the present invention relates to a method to inhibit complement receptor type 2 (CR2)-dependent human immunodeficiency virus-1 (HIV-1) infection of cells in a patient. This method includes the steps of administering to a patient infected with HIV-1 an inhibitor compound that inhibits the binding of C3d, C3 or another CR2-binding fragment of C3 containing C3d or a portion thereof, -opsonized HIV-1 to B cells, follicular dendritic cells, T cells or macrophages in the patient. The inhibitor compound is selected by the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as previously described herein; (b) identifying a candidate compound for binding to said CR2 SCR 1-2 region by performing structure based drug design with said structure of (a) to identify a compound structure that binds to said three dimensional structure of said CR2 SCR 1-2 region; (c) contacting said candidate compound identified in step (b) with a B cell, follicular dendritic cell, T cell or macrophage expressing CR2 or a fragment thereof and C3d or a fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, under conditions in which said C3d or fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, can bind to CR2 and enhance activation of the B cell, follicular dendritic cell, T cell or macrophage in the absence of said candidate compound; and (d) measuring the activation of the B cell, follicular dendritic cell, T cell or macrophage, wherein a candidate inhibitor compound is selected as a compound that inhibits activation of the B cell, follicular dendritic cell, T cell or macrophage, as compared to in the absence of said candidate inhibitor compound.

CR2 has been shown to mediate the interaction of C3d-bound HIV-1, or HIV-1 bound to other CR2-binding C3 fragments that contain C3d or a portion thereof, as an immune complex with B cells in a fashion that promotes transfer of virus and infection of CD4 T cells (S. Moir, et al., *J Exp Med* 192, 637-46 (2000)). Therefore, it would be desirable to design or identify compounds that inhibit the interaction of C3d, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof with CR2 on B cells,

follicular dendritic cells, T cells and macrophages to reduce the infection of CD4 T cells by HIV-1. In this embodiment, the step of contacting the candidate compound identified in step (b) with a B cell, follicular dendritic cell, T cell or macrophage, expressing CR2 or a fragment thereof and C3d or a fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, occurs under conditions in which the C3d or fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, can bind to CR2 and enhance activation of the B cell, follicular dendritic cell, T cell or macrophage in the absence of the candidate compound. Such conditions have been described in detail above. In addition, the step of measuring the activation of the B cell, follicular dendritic cell, T cell or macrophage expressing CR2 (i.e., by measuring a biological activity effected by CR2) have been described above.

Once a compound has been identified that inhibits the interaction between C3d and CR2 on B cells, follicular dendritic cells, T cells and/or macrophages, the compound is administered to a patient infected with HIV-1. A preferred patient to treat includes a patient with early-onset HIV infection. Such a patient can be defined herein as a patient that meets one or more of the following criteria: (1)the patient has a blood $CD4^+$ T cell count of at least about 100 cells/mm^3, and preferably, at least about 200 cells/mm^3, and more preferably, at least about 300 cells/mm^3, and even more preferably, at least about 400 cells/mm^3 as determined within 30 days of the time of employment of the present method; and (2) the patient has an HIV serum load of less than about 400 copies/ml, and preferably, less than about 300 copies/ml, and more preferably, less than about 200 copies/ml, and even more preferably, less than about 100 copies/ml, and most preferably undetectable viral load, as determined by plasma RNA PCT within 30 days of when the method is employed. In one embodiment, the patient is characterized as having a $CD4^+$ T cell count of at least about 100 cells/mm^3 when the method is employed and/or an HIV viral load of less than about 400 copies/ml when the method is employed.

A composition to be administered to a patient, such as in this embodiment, generally includes the compound identified by the structure based identification method and a carrier, and preferably, a pharmaceutically acceptable carrier. According to the present invention, a "pharmaceutically acceptable carrier" includes pharmaceutically acceptable excipients and/or pharmaceutically acceptable delivery vehicles, which are suitable for use in administration of the composition to a suitable *in vitro*, *ex vivo* or *in vivo* site. A suitable *in vitro*, *in vivo* or *ex vivo* site is preferably at or near a cell that expresses a CR2, and most preferably, at or near a site of interest in the patient. Preferred pharmaceutically acceptable carriers are capable of maintaining a compound identified by the present methods in a form that, upon arrival of compound at the cell target in a culture or in patient, the compound is capable of interacting with its target (e.g., a CR2).

Suitable excipients of the present invention include excipients or formularies that transport or help transport, but do not specifically target a composition to a cell (also referred to herein as non-targeting carriers). Examples of pharmaceutically acceptable excipients include, but are not limited to water, phosphate buffered saline, Ringer's solution, dextrose solution, serum-containing solutions, Hank's solution, other aqueous physiologically balanced solutions, oils, esters and glycols. Aqueous carriers can contain suitable auxiliary substances required to approximate the physiological conditions of the recipient, for example, by enhancing chemical stability and isotonicity.

Suitable auxiliary substances include, for example, sodium acetate, sodium chloride, sodium lactate, potassium chloride, calcium chloride, and other substances used to produce phosphate buffer, Tris buffer, and bicarbonate buffer. Auxiliary substances can also include preservatives, such as thimerosal, — or o-cresol, formalin and benzol alcohol. Compositions of the present invention can be sterilized by conventional methods and/or lyophilized.

One type of pharmaceutically acceptable carrier includes a controlled release formulation that is capable of slowly releasing a composition of the present invention into a patient or culture. As used herein, a controlled release formulation comprises a compound

of the present invention (e.g., a protein (including homologues), a drug, an antibody, a nucleic acid molecule, or a mimetic) in a controlled release vehicle. Suitable controlled release vehicles include, but are not limited to, biocompatible polymers, other polymeric matrices, capsules, microcapsules, microparticles, bolus preparations, osmotic pumps, diffusion devices, liposomes, lipospheres, and transdermal delivery systems. Other carriers of the present invention include liquids that, upon administration to a patient, form a solid or a gel *in situ*. Preferred carriers are also biodegradable (i.e., bioerodible). When the compound is a recombinant nucleic acid molecule, suitable delivery vehicles include, but are not limited to liposomes, viral vectors or other delivery vehicles, including ribozymes. Natural lipid-containing delivery vehicles include cells and cellular membranes. Artificial lipid-containing delivery vehicles include liposomes and micelles. A delivery vehicle of the present invention can be modified to target to a particular site in a patient, thereby targeting and making use of a compound of the present invention at that site. Suitable modifications include manipulating the chemical formula of the lipid portion of the delivery vehicle and/or introducing into the vehicle a targeting agent capable of specifically targeting a delivery vehicle to a preferred site, for example, a preferred cell type. Other suitable delivery vehicles include gold particles, poly-L-lysine/DNA-molecular conjugates, and artificial chromosomes.

A pharmaceutically acceptable carrier which is capable of targeting is herein referred to as a "delivery vehicle." Delivery vehicles of the present invention are capable of delivering a composition of the present invention to a target site in a patient. A "target site" refers to a site in a patient to which one desires to deliver a composition. For example, a target site can be any cell which is targeted by direct injection or delivery using liposomes, viral vectors or other delivery vehicles, including ribozymes and antibodies. Examples of delivery vehicles include, but are not limited to, artificial and natural lipid-containing delivery vehicles, viral vectors, and ribozymes. Natural lipid-containing delivery vehicles include cells and cellular membranes. Artificial lipid-containing delivery vehicles include liposomes and micelles. A delivery vehicle of the present invention can be modified to target

to a particular site in a subject, thereby targeting and making use of a compound of the present invention at that site. Suitable modifications include manipulating the chemical formula of the lipid portion of the delivery vehicle and/or introducing into the vehicle a compound capable of specifically targeting a delivery vehicle to a preferred site, for example, a preferred cell type. Specifically, targeting refers to causing a delivery vehicle to bind to a particular cell by the interaction of the compound in the vehicle to a molecule on the surface of the cell. Suitable targeting compounds include ligands capable of selectively (i.e., specifically) binding another molecule at a particular site. Examples of such ligands include antibodies, antigens, receptors and receptor ligands. Manipulating the chemical formula of the lipid portion of the delivery vehicle can modulate the extracellular or intracellular targeting of the delivery vehicle. For example, a chemical can be added to the lipid formula of a liposome that alters the charge of the lipid bilayer of the liposome so that the liposome fuses with particular cells having particular charge characteristics. In one embodiment, a targeting carrier can be a portion of a CR2 protein as described elsewhere herein, which is linked to the compound.

One preferred delivery vehicle of the present invention is a liposome. A liposome is capable of remaining stable in an animal for a sufficient amount of time to deliver a nucleic acid molecule or other compound to a preferred site in the animal. A liposome, according to the present invention, comprises a lipid composition that is capable of delivering a nucleic acid molecule or other compound to a particular, or selected, site in a patient. A liposome according to the present invention comprises a lipid composition that is capable of fusing with the plasma membrane of the targeted cell to deliver a nucleic acid molecule or other compound into a cell. Suitable liposomes for use with the present invention include any liposome. Preferred liposomes of the present invention include those liposomes commonly used in, for example, gene delivery methods known to those of skill in the art. More preferred liposomes comprise liposomes having a polycationic lipid composition and/or liposomes having a cholesterol backbone conjugated to polyethylene

glycol. Complexing a liposome with a nucleic acid molecule or other compound can be achieved using methods standard in the art.

A liposome delivery vehicle is preferably capable of remaining stable in a patient for a sufficient amount of time to deliver a nucleic acid molecule or other compound of the present invention to a preferred site in the patient (i.e., a target cell). A liposome delivery vehicle of the present invention is preferably stable in the patient into which it has been administered for at least about 30 minutes, more preferably for at least about 1 hour and even more preferably for at least about 24 hours. A preferred liposome delivery vehicle of the present invention is from about 0.01 microns to about 1 microns in size.

Another preferred delivery vehicle comprises a viral vector. A viral vector includes an isolated nucleic acid molecule useful in the present invention, in which the nucleic acid molecules are packaged in a viral coat that allows entrance of DNA into a cell. A number of viral vectors can be used, including, but not limited to, those based on alphaviruses, poxviruses, adenoviruses, herpesviruses, lentiviruses, adeno-associated viruses and retroviruses.

A composition which includes an compound identified according to the present methods can be delivered to a cell culture or patient by any suitable method. Selection of such a method will vary with the type of compound being administered or delivered (i.e., protein, peptide, nucleic acid molecule, mimetic, or other type of compound), the mode of delivery (i.e., *in vitro*, *in vivo*, *ex vivo*) and the goal to be achieved by administration/delivery of the compound or composition. According to the present invention, an effective administration protocol (i.e., administering a composition in an effective manner) comprises suitable dose parameters and modes of administration that result in delivery of a composition to a desired site (i.e., to a desired cell) and/or in the desired regulatory event (e.g., inhibition of the binding of C3d-opsonized HIV-1 to B cells or follicular dendritic cells in the patient).

Administration routes include *in vivo*, *in vitro* and *ex vivo* routes. *In vivo* routes include, but are not limited to, oral, nasal, intratracheal injection, inhaled, transdermal, rectal,

and parenteral routes. Preferred parenteral routes can include, but are not limited to, subcutaneous, intradermal, intravenous, intramuscular and intraperitoneal routes. Intravenous, intraperitoneal, intradermal, subcutaneous and intramuscular administrations can be performed using methods standard in the art. Aerosol (inhalation) delivery can also be performed using methods standard in the art (see, for example, Stribling et al., *Proc. Natl. Acad. Sci. USA* 189:11277-11281, 1992, which is incorporated herein by reference in its entirety). Oral delivery can be performed by complexing a therapeutic composition of the present invention to a carrier capable of withstanding degradation by digestive enzymes in the gut of an animal. Examples of such carriers, include plastic capsules or tablets, such as those known in the art. Direct injection techniques are particularly useful for suppressing graft rejection by, for example, injecting the composition into the transplanted tissue, or for site-specific administration of a compound, such as at the site of a tumor. *Ex vivo* refers to performing part of the regulatory step outside of the patient, such as by transfecting a population of cells removed from a patient with a recombinant molecule comprising a nucleic acid sequence encoding a protein according to the present invention under conditions such that the recombinant molecule is subsequently expressed by the transfected cell, and returning the transfected cells to the patient. *In vitro* and *ex vivo* routes of administration of a composition to a culture of host cells can be accomplished by a method including, but not limited to, transfection, transformation, electroporation, microinjection, lipofection, adsorption, protoplast fusion, use of protein carrying agents, use of ion carrying agents, use of detergents for cell permeabilization, and simply mixing (e.g., combining) a compound in culture with a target cell.

In this particular embodiment of the invention (i.e., the inhibition of HIV infection), it will be obvious to one of skill in the art that the number of doses administered to an immunodeficiency virus infected patient is dependent upon the extent of the infection and the response of an individual to the treatment. For example, in the case of HIV-infection, a patient having a high titer of HIV may require more doses than a patient having lower titers.

In some cases, however, a patient having a high titer of HIV may require fewer doses than a patient having lower titers, if the patient with the high titer responds more favorably to the therapeutic composition than the patient with the lower titer. Thus, it is within the scope of the present invention that a suitable number of doses, as well as the time periods between administration, includes any number required to cause regression of a disease.

In another embodiment, this method is employed in conjunction with administration to the patient of one or more anti-retroviral therapeutic compounds. Such compounds include, but are not limited to, AZT, ddI, ddC, d4T, 3TC and/or protease inhibitors.

Another embodiment of the present invention relates to a method of preparing a vaccine, comprising linking a compound that increases B cell activation to an antigen to form the vaccine. The compound is selected by a method including the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as previously described herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) contacting the candidate compound identified in step (b) with a B cell expressing CR2 or a fragment thereof and with C3d or a fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, under conditions in which said C3d or fragment thereof, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof, can bind to and activate CR2 in the absence of said candidate compound; and (d) measuring the activation of the B cell. A candidate compound for use in a vaccine is selected as a compound that increases B cell activation as compared to in the absence of the candidate compound.

Because CR2 plays a critical role as a coreceptor for B cells and is expressed on other cells as well, CR2 is a molecular target for adjuvants and can enhance the immune response to vaccines. Therefore, in this method, compounds are identified that bind to CR2 and that enhance B cell activation, either by enhancing the interaction between CR2 and a natural

ligand (e.g., C3d), or by directly interacting with CR2 to enhance downstream biological activities of the receptor, as previously discussed herein. Methods for contacting a cell with the compound and measuring the activation events associated with CR2 activation have been previously described. In addition, to measure B cell activation, one can measure calcium mobilization, immunoglobulin class switching, cytokine production, activation of NF-κB, activation of MAP kinases, protein kinase activity and phosphorylation of proteins associated with B cell activation. In this embodiment, the conditions under which the B cell is contacted typically include the presence of an antigen that binds to the B cell antigen receptor, in addition to the other components. A compound for use in a vaccine, once identified, is typically associated with a protein (antigen or antigen-containing composition) or nucleic acid to be administered to a patient as part of the vaccine. The use of a compound identified by the present method will potentiate the immune response to the antigen.

Another embodiment of the present invention relates to a drug delivery system that will preferentially deliver compounds to sites of complement activation containing CR2-binding fragments of C3 (e.g., C3 and portions thereof that contain C3d). Such a drug delivery system includes: (a) a drug; and, (b) a portion of a CR2 protein that includes one or more of: (i) a portion comprising positions on strand B and the B-C loop of SCR2 including: G79-G80-Y81-K82-I83-R84-G85-S86-T87-P88-Y89; (ii) a portion comprising position K100 on the B strand of CR2; and, (iii) a portion comprising positions: V130-F131-P132-L133 (positions given with reference to SEQ ID NO:4). In one embodiment, the portion of the CR2 protein can also contain positions T101-N102-F103 (reference again to SEQ ID NO:4). The drug is linked to the portion of CR2 by any suitable method, covalently or non-covalently, including by recombinant means or by chemical means. In this embodiment, the CR2 is not a full-length protein, or the soluble form of CR2, as it is known in the art (i.e., the natural soluble CR2 or the CR2 with the membrane portion removed), but rather, includes less of the amino acid sequence than the full-length or the soluble CR2, and preferably, just the portions of SCR1 and SCR2 that have been determined herein to be involved in the

contact between CR2 and a natural ligand (e.g., C3d) and that are required to form a CR2 portion with the tertiary structure necessary to bind to C3d (or a fragment thereof). Therefore, the portion of CR2 used in the drug delivery system consists essentially of at least one or more of the above-recited segments of CR2, including a contiguous segment containing all of the segments (i.e., from positions 79-133 of SEQ ID NO:4), and has the three dimensional conformation of CR2 at the CR2-C3d interface, such that the portion will bind to C3d, C3 or other CR2-binding fragments of C3 that contain C3d or a portion thereof. Therefore, the portion of CR2 suitable for use in a drug delivery system includes the portions of CR2 that contact C3d, as well as the portions required to maintain the spatial positions of the contact residues, such that the tertiary structure of the C3d binding portion is conformationally similar to the tertiary structure of the C3d binding portion of the CR2 crystal described herein, using the parameters for structural homologues as described elsewhere herein for the structure of the CR2 complexed with C3d. According to the present invention, a CR2 fragment consisting essentially of the portions of SCR1 and SCR2 that have been determined herein to be involved in the contact between CR2 and C3d can have at least one, and up to about 20 (in whole number increments), additional heterologous amino acids flanking each of the C- and/or N-terminal end of the CR2 portion that contains the above-described segments and the sequence necessary to maintain the appropriate tertiary structure to bind to C3d (or a fragment thereof). According to the present invention, the heterologous amino acids are a sequence of amino acids that are not naturally found (i.e., not found in nature, *in vivo*) flanking the CR2 sequence that makes up the portion of CR2 or which would not be encoded by the nucleotides that flank the naturally occurring CR2 nucleic acid sequence as it occurs in the gene, if such nucleotides in the naturally occurring sequence were translated using standard codon usage for the organism from which the given CR2 portion is derived. Such heterologous amino acids can include a sequence that is less than about 75% similar to the natural sequence in the same positions. This embodiment also includes methods of identifying such portions of CR2.

Drugs that are desirable to deliver using the drug delivery system of the present invention include any drug that may have a beneficial effect on a subject when delivered to a site of complement activation wherein C3 and/or CR2-binding portions of C3 are present. The drugs can be protein-based, carbohydrate-based, lipid-based, nucleic acid-based, or any small molecule. Examples of such drugs include, but are not limited to, anti-inflammatory compounds, cytotoxic drugs, complement regulatory proteins, corticosteroids, and any compounds useful in ischemic, inflammatory autoimmune or vascular diseases, all of which have C3 fragments present.

In this embodiment, drug design strategies as specifically described above with regard to the identification of compounds that bind to CR2 and affect its interaction with various ligands can be similarly applied to the CR2 structure itself. CR2 proteins designed by this method can be used as drug delivery vehicles or to otherwise alter the biological activity of a CR2, such as by competing for a naturally occurring CR2 *in vivo*. One of ordinary skill in the art, using the art recognized modeling programs and drug design methods, many of which are described herein, to prepare portions of complement receptor type 2 (CR2) proteins that bind to their ligands, including CR2 homologues that retain ligand binding activity. In addition, one of skill in the art can produce CR2 proteins having modified biological activity. For example, such a method can include: (a) providing a three dimensional structure of a CR2 SCR1-2 domain as previously described herein; (b) analyzing the three dimensional structure to the three-dimensional structure of the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to the sites in the structure contributing to ability of CR2 to bind to a ligand (e.g., C3d or other CR2-binding fragments of C3); and (c) producing a protein that is a portion of CR2 that includes such sites. In the method to produce a CR2 protein having modified biological activity, one can analyze the three dimensional structure of CR2 provided herein to identify at least one site that contributes to the biological activity of the protein, and then modify at least one such site to alter the biological activity of the CR2 protein. Methods to altered proteins for CR2 biological

activity include testing the altered protein for any of the biological activities of CR2 previously described herein.

Another embodiment of the present invention relates to an antibody that selectively binds to CR2. The antibody binds to a portion of CR2 selected from the group consisting of: (a) the interface between the SCR1 and SCR2 domains of CR2; (b) the dimer interface between two CR2 proteins; and, (c) the interface between CR2 and C3d (where the C3d includes any CR2-binding fragments of C3 that contain C3d or a portion thereof). The portion of the CR2-C3d interface bound by the antibody preferably includes at site selected from: (a) the B strand and the B-C loop of CR2 SCR2 comprising the segment: G79-G80-Y81-K82-I83-R84-G85-S86-T87-P88-Y89; (b) the B strand of CR2 SCR2 comprising position K100; and (c) a segment of CR2 SCR2 comprising V130-F131-P132-L133. Prior to the present invention, the three dimensional structure of the CR2 interfaces set forth above were not known and therefore, it was not possible to design or identify an antibody by making use of such structural information. The present inventors have provided suitable target sites, including specific residues within such sites, for the design and identification of antibodies.

According to the present invention, the phrase "selectively binds to" refers to the ability of an antibody, antigen binding fragment or binding partner of the present invention to preferentially bind to specified proteins (e.g., the recited portions of a CR2 of the present invention). More specifically, the phrase "selectively binds" refers to the specific binding of one protein to another (e.g., an antibody, fragment thereof, or binding partner to an antigen), wherein the level of binding, as measured by any standard assay (e.g., an immunoassay), is statistically significantly higher than the background control for the assay. For example, when performing an immunoassay, controls typically include a reaction well/tube that contain antibody or antigen binding fragment alone (i.e., in the absence of antigen), wherein an amount of reactivity (e.g., non-specific binding to the well) by the antibody or antigen binding fragment thereof in the absence of the antigen is considered to

be background. Binding can be measured using a variety of methods standard in the art including enzyme immunoassays (e.g., ELISA), immunoblot assays, etc.

Limited digestion of an immunoglobulin with a protease may produce two fragments. An antigen binding fragment is referred to as an Fab, an Fab', or an $F(ab')_2$ fragment. A fragment lacking the ability to bind to antigen is referred to as an Fc fragment. An Fab fragment comprises one arm of an immunoglobulin molecule containing a L chain ($V_L + C_L$ domains) paired with the V_H region and a portion of the C_H region (CH1 domain). An Fab' fragment corresponds to an Fab fragment with part of the hinge region attached to the CH1 domain. An $F(ab')_2$ fragment corresponds to two Fab' fragments that are normally covalently linked to each other through a di-sulfide bond, typically in the hinge regions.

Functional aspects of an immunoglobulin molecule include the valency of an immunoglobulin molecule, the affinity of an immunoglobulin molecule, and the avidity of an immunoglobulin molecule. As used herein, affinity refers to the strength with which an immunoglobulin molecule binds to an antigen at a single site on an immunoglobulin molecule (i.e., a monovalent Fab fragment binding to a monovalent antigen). Affinity differs from avidity which refers to the sum total of the strength with which an immunoglobulin binds to an antigen. Immunoglobulin binding affinity can be measured using techniques standard in the art, such as competitive binding techniques, equilibrium dialysis or BIAcore methods. As used herein, valency refers to the number of different antigen binding sites per immunoglobulin molecule (i.e., the number of antigen binding sites per antibody molecule of antigen binding fragment). For example, a monovalent immunoglobulin molecule can only bind to one antigen at one time, whereas a bivalent immunoglobulin molecule can bind to two or more antigens at one time, and so forth. Both monovalent and bivalent antibodies that selectively bind to CR2 of the present invention are encompassed herein.

In one embodiment of the present invention, a monovalent antibody can be used as a regulatory compound. Such an antibody is not capable of aggregating receptors. Divalent antibodies can also be used in the present invention.

In one embodiment, the antibody is a bi- or multi-specific antibody. A bi-specific (or multi-specific) antibody is capable of binding two (or more) antigens, as with a divalent (or multivalent) antibody, but in this case, the antigens are different antigens (i.e., the antibody exhibits dual or greater specificity). A bi-specific antibody suitable for use in the present method includes an antibody having: (a) a first portion (e.g., a first antigen binding portion) which binds to CR2; and (b) a second portion which binds to a cell surface molecule expressed by a cell which expresses CR2. In this embodiment, the second portion can bind to any cell surface molecule. In a preferred embodiment, the second portion is capable of targeting the regulatory antibody to a specific target cell (i.e., the regulatory antibody binds to a target molecule).

Isolated antibodies of the present invention can include serum containing such antibodies, or antibodies that have been purified to varying degrees. Whole antibodies of the present invention can be polyclonal or monoclonal. Alternatively, functional equivalents of whole antibodies, such as antigen binding fragments in which one or more antibody domains are truncated or absent (e.g., Fv, Fab, Fab', or $F(ab)_2$ fragments), as well as genetically-engineered antibodies or antigen binding fragments thereof, including single chain antibodies or antibodies that can bind to more than one epitope (e.g., bi-specific antibodies), or antibodies that can bind to one or more different antigens (e.g., bi- or multi-specific antibodies), may also be employed in the invention.

Genetically engineered antibodies of the invention include those produced by standard recombinant DNA techniques involving the manipulation and re-expression of DNA encoding antibody variable and/or constant regions. Particular examples include, chimeric antibodies, where the V_H and/or V_L domains of the antibody come from a different source to the remainder of the antibody, and CDR grafted antibodies (and antigen binding fragments thereof), in which at least one CDR sequence and optionally at least one variable region framework amino acid is (are) derived from one source and the remaining portions of the variable and the constant regions (as appropriate) are derived from a different source.

Construction of chimeric and CDR-grafted antibodies are described, for example, in European Patent Applications: EP-A 0194276, EP-A 0239400, EP-A 0451216 and EP-A 0460617.

Alternative methods, employing, for example, phage display technology (see for example US 5969108, US 5565332, US 5871907, US 5858657) or the selected lymphocyte antibody method of US 5627052 may also be used for the production of antibodies and/or antigen fragments of the invention, as will be readily apparent to the skilled individual.

Generally, in the production of an antibody, a suitable experimental animal, such as, for example, but not limited to, a rabbit, a sheep, a hamster, a guinea pig, a mouse, a rat, or a chicken, is exposed to an antigen against which an antibody is desired. Typically, an animal is immunized with an effective amount of antigen that is injected into the animal. An effective amount of antigen refers to an amount needed to induce antibody production by the animal. The animal's immune system is then allowed to respond over a pre-determined period of time. The immunization process can be repeated until the immune system is found to be producing antibodies to the antigen. In order to obtain polyclonal antibodies specific for the antigen, serum is collected from the animal that contains the desired antibodies (or in the case of a chicken, antibody can be collected from the eggs). Such serum is useful as a reagent. Polyclonal antibodies can be further purified from the serum (or eggs) by, for example, treating the serum with ammonium sulfate.

Monoclonal antibodies may be produced according to the methodology of Kohler and Milstein (*Nature* 256:495-497, 1975). For example, B lymphocytes are recovered from the spleen (or any suitable tissue) of an immunized animal and then fused with myeloma cells to obtain a population of hybridoma cells capable of continual growth in suitable culture medium. Hybridomas producing the desired antibody are selected by testing the ability of the antibody produced by the hybridoma to bind to the desired antigen.

Another embodiment of the present invention relates to a therapeutic composition that, when administered to an animal, enhances B cell responses in the animal. The

therapeutic composition includes a compound that stimulates the activity of a complement receptor type 2 (CR2), which has been identified by a method of structure based identification of compounds of the present invention, as described in detail above. Specifically, this method includes the steps of: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as described previously herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) synthesizing the candidate compound; and (d) selecting candidate compounds that bind to and activate CR2.

Another embodiment of the present invention relates to a therapeutic composition that, when administered to an animal, inhibits the biological activity of complement receptor type 2 (CR2) in the animal. The therapeutic composition comprises a compound that inhibits the activity of a complement receptor type 2 (CR2), the compound being identified by the method comprising: (a) providing a three dimensional structure of a CR2 short consensus repeat (SCR) 1-2 region as previously described herein; (b) identifying a candidate compound for binding to the CR2 SCR 1-2 region by performing structure based drug design with the structure of (a) to identify a compound structure that binds to the three dimensional structure of the CR2 SCR 1-2 region; (c) synthesizing the candidate compound; and (d) selecting candidate compounds that inhibit the biological activity of CR2. Preferably, the compounds inhibit the formation of a complex between CR2 and a CR2 ligand, such ligand including, but not limited to, C3d, CD23 and Epstein Barr Virus (EBV). In a more preferred embodiment, the compound inhibits the activation of CR2.

Methods of identifying candidate compounds and selecting compounds that bind to and activate or inhibit CR2 have been previously described herein. Candidate compounds can be synthesized using techniques known in the art, and depending on the type of compound. Synthesis techniques for the production of non-protein compounds, including organic and inorganic compounds are well known in the art.

For smaller peptides, chemical synthesis methods are preferred. For example, such methods include well known chemical procedures, such as solution or solid-phase peptide synthesis, or semi-synthesis in solution beginning with protein fragments coupled through conventional solution methods. Such methods are well known in the art and may be found in general texts and articles in the area such as: Merrifield, 1997, *Methods Enzymol.* 289:3-13; Wade et al., 1993, *Australas Biotechnol.* 3(6):332-336; Wong et al., 1991, *Experientia* 47(11-12):1123-1129; Carey et al., 1991, *Ciba Found Symp.* 158:187-203; Plaue et al., 1990, *Biologicals* 18(3):147-157; Bodanszky, 1985, *Int. J. Pept. Protein Res.* 25(5):449-474; or H. Dugas and C. Penney, BIOORGANIC CHEMISTRY, (1981) at pages 54-92, all of which are incorporated herein by reference in their entirety. For example, peptides may be synthesized by solid-phase methodology utilizing a commercially available peptide synthesizer and synthesis cycles supplied by the manufacturer. One skilled in the art recognizes that the solid phase synthesis could also be accomplished using the FMOC strategy and a TFA/scavenger cleavage mixture.

If larger quantities of a protein are desired, or if the protein is a larger polypeptide, the protein can be produced using recombinant DNA technology. A protein can be produced recombinantly by culturing a cell capable of expressing the protein (i.e., by expressing a recombinant nucleic acid molecule encoding the protein) under conditions effective to produce the protein, and recovering the protein. Effective culture conditions include, but are not limited to, effective media, bioreactor, temperature, pH and oxygen conditions that permit protein production. An effective medium refers to any medium in which a cell is cultured to produce the protein. Such medium typically comprises an aqueous medium having assimilable carbon, nitrogen and phosphate sources, and appropriate salts, minerals, metals and other nutrients, such as vitamins. Recombinant cells (i.e., cells expressing a nucleic acid molecule encoding the desired protein) can be cultured in conventional fermentation bioreactors, shake flasks, test tubes, microtiter dishes, and petri plates. Culturing can be carried out at a temperature, pH and oxygen content appropriate for a

recombinant cell. Such culturing conditions are within the expertise of one of ordinary skill in the art. Such techniques are well known in the art and are described, for example, in Sambrook et al., 1988, Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Press, Cold Spring Harbor Laboratory, Cold Spring Harbor, New York or Current Protocols in Molecular Biology (1989) and supplements.

As discussed above, a composition, and particularly a therapeutic composition, of the present invention generally includes the therapeutic compound (e.g., the compound identified by the structure based identification method) and a carrier, and preferably, a pharmaceutically acceptable carrier. Pharmaceutically acceptable carriers and preferred methods of administration of therapeutic compositions of the present invention have been described in detail above with regard to the administration of an inhibitor compound to a patient infected with HIV. Such carriers and administration protocols are applicable to this embodiment.

Yet another embodiment of the present invention relates to an isolated C3d mutant protein, C3 or other CR2-binding fragments of C3 that contain a mutant C3d or a portion thereof, comprising an amino acid substitution of an non-asparagine amino acid residue at position 170 wherein said C3d mutant protein, C3 or other CR2-binding fragments of C3 that contain the mutant C3d or a portion thereof, has reduced binding to complement receptor type 2 (CR2), as compared to a wild-type C3d protein (SEQ ID NO:7), or equivalent wild-type CR2-binding fragment of C3 that contain C3d or a portion thereof. Preferably, the mutant protein is at least about 50% identical to SEQ ID NO:7, and more preferably at least about 60% identical, and more preferably at least about 70% identical, and more preferably at least about 80% identical, and more preferably at least about 90% identical, and more preferably at least about 95% identical to SEQ ID NO:7. In a preferred embodiment, the mutant protein comprises SEQ ID NO:8 (mt170 or mut2) or SEQ ID NO:9 (mut4).

Another embodiment of the present invention relates to a computer for producing a three-dimensional model of a molecule or molecular structure, wherein the molecule or molecular structure comprises a three dimensional structure defined by atomic coordinates

of a complement receptor type 2 (CR2) protein, according to Table 2 or Table 3, or a three-dimensional model of a homologue of the molecule or molecular structure, wherein the homologue comprises a three dimensional structure that has an average root-mean-square deviation (RMSD) of equal to or less than about 1.0 Å for the backbone atoms in secondary structure elements in the CR2 protein, wherein the computer comprises:

a. a computer-readable medium encoded with the atomic coordinates of the CR2 protein, according to Table 2 or Table 3, to create an electronic file;

b. a working memory for storing a graphical display software program for processing the electronic file;

c. a processor coupled to the working memory and to the computer-readable medium which is capable of representing the electronic file as the three dimensional model; and,

d. a display coupled to the processor for visualizing the three dimensional model;

wherein the three dimensional structure of the CR2 protein is displayed on the computer.

The following examples are provided for the purpose of illustration and are not intended to limit the scope of the present invention.

EXAMPLES

Example 1

The following example describes the crystallization and structure determination of the complex of complement receptor type 2 (CR2) and C3d.

Crystallization and Structure Determination of Structure

The crystals of the complex of CR2-C3d were obtained by co-crystallization of CR2 and C3d, at a protein ratio where no free CR2 or C3d could be detected by native gel

electrophoresis. The protein concentration of 20 mg/ml was used for crystallization by the method of hanging drop vapor diffusion. The crystallization buffer contained 17% PEG 2K, 0.2 M ZnAcetate, and 0.1 M NaCacodylate (pH 7.36). Crystals reached full size after 4-6 weeks at 4°C. Crystal was frozen under liquid nitrogen in the crystallization buffer containing 20% glycerol. Synchrotron data were collected at Brookhaven National Laboratory and was indexed, integrated and reduced using D*trek (licensed through MSC Inc., Table 1). The space group is R32, with unit cell a=b=170.5Å, c=173.8 Å. AmoRe (CCP4, *Acta Cryst.* D50, 760-763 (1994)) was used to do molecular replacement that was carried out using C3d (Accession No. 1C3D from the Protein Data Bank (PDB)) as a search model. The final correlation function and R factor after rotation and translation search were 50% and 45%. Initial phase improvement was carried out using solvent flattening and two fold averaging by the program DM (CCP4, *Acta Cryst.* D50, 760-763 (1994)) in CCP4 suit. Stepwise model building and refinement were carried out using program "O" and CNS (P. D. A. A.T.Brunger, G.M.Clore, W.L.Delano, P.Gros, R.W.Grosse-Kunstleve, J.-S.Jiang, J.Kuszewski, N. S. P. M.Nilges, R.J.Read, L.M.Rice, T.Simonson, G.L.Warren, *Acta Cryst.* D54, 905-921 (1998)). The final complete model was refined using simulated annealing, positional refinement, and individual B factor refinement. Water molecules were added last using CNS (Table 1).

Table 1. Structure determination and refinement	
Data collection statistics	
Space group	R32
Unit cell length (Å)	a=b=170.5, c=173.8
Resolution (Å)	25.0-2.04
Completeness (last bin)	94.1 / 83.6
Total reflections	255801
Unique reflections	63919
[1] Rsym (last bin)%	6.7 / 22.3
I/δ (last bin)	10.8 / 3.7
Refinement statistics	
% of reflections for R_{free}	10
R_{work}/R_{free}	20.8 / 23.9
rmsd from ideality	
Bond length (Å)	0.006
Bond angle (°)	1.10
Dihedral angle (°)	16.8
Ramachandran plot (core, disallowed)	92.3 / 0
Average B factor	33.98
rmsd of B factor (Å^2)	1.2
Protein atoms in the model	8878
H_2O in the model	580

[1] Rsym = $\sum_{ij} |I(j) - \langle I(j) \rangle| / \sum_{ij} I_i(j)$, where $I_i(j)$ is the i-th measurement of reflection j and $\langle I(j) \rangle$ is the overall weighted mean of j measurements.

The atomic coordinates representing the structure of the complex of CR2 and C3d were deposited on January 11, 2001, with the Protein Data Bank (PDB), operated by the Research Collaboratory for Structural Bioinformatics (RCSB) (H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne, The Protein Data Bank: *Nucleic Acids Research*, 28:235-242 (2000)), under PDB Deposit No. PDB id 1GHQ. These atomic coordinates are also represented herein as Table 2.

Description of the overall structure of the CR2-C3d complex

Figs. 1A and 1B show the structure of the CR2 -C3d complex. Fig. 1A is an overall view of the structure of CR2 binding to C3d, showing only SCR2 contacting one portion of the edge of C3d. CR2 SCR1 is colored in red and SCR2 in yellow, while C3d is in cyan. The side chain of residue Q20 of C3d that forms an ester-bond with antigen is drawn in pink and labeled. The position of residue D223 of C3d, which is the C3F form (fast migrating variant on agarose gel electrophoresis) that is associated with an increased incidence of certain diseases (M. C. Poznansky et al., *J Immunol* 143, 1254-8 (1989)), is also labeled. The other form of C3d, C3S (slow migration), has an N223 residue. The N and C termini of C3d (N1 and C307, respectively) are positioned next to each other. Fig. 1B shows the overall structure showing a second CR2-C3d complex (colored in light blue and grey) that dimerizes with the first one in Fig. 1A. The dimerization contact in the two-complex structure is through SCR1 of CR2 at the very top. (Prepared with the program MOLSCRIPT).

The complex contains a V-shaped CR2 receptor binding to a globular C3d ligand (Fig. 1A). The CR2 receptor portion contains two domains (SCR1 and SCR2) that pack against each other almost side to side, producing a drastic bend of 53 degrees between the two domains to give a V-shape. A well-structured linker of 8 amino acids (residues 64-71) connects the SCR1 and SCR2 domains. Both SCR1 and SCR2 domains consist of only beta-strands and coils, which is characteristic of the SCR fold that contains a beta-barrel core structure (A. P. Wiles, et al., *J Mol Biol* 272, 253-65 (1997); P. N. Barlow, et al., *J Mol Biol* 232, 268-84 (1993); J. M. Casasnovas, M. Larvie, T. Stehle, *EMBO J* 18, 2911-22 (1999); R. Schwarzenbacher, et al., *EMBO J* 18, 6228-39 (1999)). The V-shaped two-domain CR2 molecule has a span of 42.6 Å at the base of the molecule (from SCR1 to SCR2), and the height of "V" structure (from base to tip) measures 38.5 Å.

The C3d ligand, which has a dome-shaped structure that consists of mostly alpha helices (B. Nagar, R. G. Jones, R. J. Diefenbach, D. E. Isenman, J. M. Rini, *Science* 280, 1277-81 (1998)), interacts with the receptor using one portion of the edge of the dome. The

CR2-contact edge of C3d is located on nearly the opposite side of the amino (N) and carboxyl (C) termini, which are physically proximate to each other (Fig. 1A). Binding to CR2 through this edge leaves the concave and convex surfaces free and the rest of the iC3b molecule (a form of C3 encompassing the C3d domain with which CR2 also interacts) likely oriented away from CR2 (Fig. 1A). The site of the ester-bond linkage to antigens (Q20) sits approximately half way between the receptor contact edge and the N and C termini of C3d (Fig. 1A). The site of mutation (N223 to D223, Fig. 1A) that defines an important disease-related allelic polymorphism, C3F (fast) versus C3S (slow) (M. C. Poznansky, P. M. Clissold, P. J. Lachmann, *J Immunol* 143, 1254-8 (1989)), is located away from the CR2 interaction site; therefore, this disease association is likely not directly related to CR2 binding but rather to other C3 functions.

Unexpectedly, a dimer of CR2 molecules is formed in the crystal through contacts between SCR1 domains (Fig. 1B). This CR2 dimer has a shape of two letter V's coming together head to head, with SCR1 facing SCR1 and SCR2 facing SCR2. No direct contacts occur between SCR2. This second CR2 is essentially a duplicate of the other CR2 molecule of the dimer that binds to C3d (Fig. 1B).

Description of the structure of CR2

Figs 2A-2E show the structure of CR2. Fig. 2A is a ribbon representation of the CR2 SCR1 (in red) and SCR2 (in yellow) structures, showing the SCR fold and the packing of the two domains to form a V shape. The side chains of Cys residues that form intra-domain disulfide bonds are colored in cyan. Within each domain, the beta-strands B-E are labeled. A sugar residue GlcNAc (N-acetyl-glucosamine) is seen attached to N102 of SCR2. (Prepared using MOLSCRIPT). Fig. 2B shows the structure and packing interaction at the interface of CR2 SCR1 and SCR2 domains. Residues important for the tight packing between the two domains at the interface and the linker regions are shown (Prepared with the program RIBBONS). Fig. 2C is a surface representation of the two-domain arrangement of CR2. (Prepared using GRASP). Fig. 2D shows the dimerization of CR2 through

interactions between SCR1 of each molecule. Strand D2 and E1 of one CR2 molecule (red) packed against strand E1 and D2 of the second CR2 molecule in the dimer (blue). (Prepared using MOLSCRIPT). Fig. 2E shows a sequence alignment between human CR2 (SEQ ID NO:4) and mouse CR2 (mCR2) (SEQ ID NO:6). The first residue of CR2 (Gly) is changed to Ala in the structure due to PCR primer sequence. Secondary structure elements are shown above the corresponding aligned sequences. A black line represents coils and arrows represent beta-strands. The linker sequence between SCR1 and SCR2 is underlined. The residues whose side-chain or main-chain groups are involved in binding to C3d are indicated by *. The symbol • indicates the two residues that, after mutating from mouse to human sequence, allow mCR2 to gain the ability to bind EBV gp350/220.

The CR2 structure described here contains residues 1-134 (SEQ ID NO:4; Fig. 2E, corresponding to residues 20-153 of the full length human CR2 (SEQ ID NO:1)) that fold into two SCR domains (Fig. 2A). Each domain shows a basic SCR fold: four anti-parallel beta-strands form a barrel-like beta-sheet. Strand D and E are separated into two segments, D1, D2 and E1, E2. In addition to the hydrogen bonds that hold together the antiparallel beta-strands, two intra-domain disulfide bonds cross-link the coiled N-terminus to strand D2, and strand C to strand E2 (Fig. 2A). A well ordered N-linked GlcNAc (N-acetyl-glucosamine) residue is linked to Asn102 that is located at the tip of SCR2. The rest of the sugar residues were digested away by EndoH.

A very unique feature of the two domain CR2 structure is that the 8 amino acid linker makes a dramatic turn to allow the two SCR domains to pack against each other sideways (Figs. 2A, 2B, 2C). Among the protein family containing SCR domains, the linkers connecting SCR domains are normally 3-5 amino acids in length, while an 8 amino acid linker is the longest known so far. The available structures of four SCR proteins containing two or 4 repeats (A. P. Wiles, et al.,(1997), *supra*; P. N. Barlow, et al., (1993), *supra*; J. M. Casasnovas, et al.,(1999), *supra*; R. Schwarzenbacher et al., (1999), *supra*) all have end-end

packing between consecutive SCRs, and CR2 is thus the first to demonstrate extensive side-side packing.

In end-end packing, the adjacent domains could, in principle, adopt different rotations and bend angles relative to each other in different environments. Indeed, a commonly held concept is that SCRs are not absolutely fixed relative to each other but rather are allowed some freedom to move about this interface (P. N. Barlow, et al., (1993), *ibid.*; J. M. Casasnovas, et al.,(1999), *ibid.*). However, the side-side packing of the CR2 SCR1 and SCR2 would not give the two domains freedom to adopt different orientations, unless some active process is involved to first separate the two domains. The interface between the two domains is mainly hydrophobic (Fig. 2B). Trp112, which is unique to CR2 SCR2 sequence and located on strand D2, plays a critical role in the packing by interacting with Ile39 and the main-chain from SCR1. Trp112 would be unfavorably exposed to the solvent if the two domains do not pack against each other sideways in this manner. In addition to Trp112, several other residues also play a role in the packing, including Pro121, His91, Leu39, and the carbon side chain of Glu64. The 8 amino acid linker, which contains mainly hydrophobic residues such as Tyr65, Phe66, Tyr69, also participates in the hydrophobic packing outside the two-domain interface, further solidifying the interactions between SCR1 and SCR2 (Fig. 2B). The area of the interface of the two SCRs is very extensive, covering almost half of the length of one SCR domain (Fig. 2C). Because of the above mentioned observations of other SCR proteins studied in the absence of their ligands, it will be interesting to see if the packing of these two CR2 SCR domains remains the same in the unliganded crystal and solution states.

Two CR2 molecules dimerize through SCR1 SCR1 contacts in the crystal structure (Fig. 2D). The contact is symmetrical, with the E1 strands from different molecules running anti-parallel to each other. The C-terminus of the E1 strand also contacts the C-terminus of the D2 strand of another molecule. The nature of the interaction is hydrogen bonds. In solution, however, the present inventors have found that CR2 behaves like a monomer under

physiological buffer condition as assayed by gel filtration chromatography, though this is a technique that can only detect strong protein-protein interaction. It is possible that the dimer interaction only occurs in the crystal packing and is not of relevance. Another possibility, though, is that the interaction plays biological roles under physiologic conditions, but it is too weak to be detected in solution. Considering that CR2 receptors are largely constrained in the cell membrane to only lateral movement, no strong interactions would be necessary to dimerize.

Description of the structure of the CR2-C3d interface

Figs. 3A-3F show the structure at the CR2-C3d interface. Figs. 3A and 3B show the surface features of the interface area on C3d (in cyan) and CR2 molecule (in yellow). The shape of the interface of one molecule complements that of the other. (Prepared using GRASP). Fig. 3C shows the structure of the CR2 SCR2-C3d complex. The strands of CR2 (yellow) and helices of C3d (cyan) near the interface are labeled to provide a sense of orientation. (Prepared using MOLSCRIPT). Figs. 3D and 3E show the detailed interactions between CR2 (in yellow) and C3d (in cyan) in two angles. Dashed lines represent hydrogen bonds between carbonyl oxygen atoms (in red), nitrogen atoms (in blue) of amino acid side chains or main chain, and water molecules (in purple). (Prepared using RIBBONS). Fig. 3F shows the human C3d sequence (SEQ ID NO:7) with secondary structure assigned on top of the corresponding sequences. The residues involved in CR2 binding are indicated by *. The residue D223 in C3F from (vs. N223 in C3S) is in pink. The residue N170 shown to weaken C3d-CR2 interaction after being mutated to Arg (see Fig. 4) is colored in red. N170 is also the only residue among those involved in CR2 binding that has its side chain in close contact with and pointing toward CR2.

One particularly salient feature of the interface is the shape-matching between C3d and CR2 interacting surfaces, as the protrusions on one molecule exactly match the pits and cavities on the other (Figs. 3A & 3B). The total of the buried area in the interface is 1400 A^2. The contact interfaces between the receptor and C3d are neither hydrophobic nor

particularly charged, but rather the well-fitted surface shapes from the two molecules come together to form the bonding contact in the complex. No major conformational difference is observed between the structures of free C3d and CR2-bound C3d, except for small movements (0.7-1.0 Å) of H3 (helix 3), H5, H7 and a few turns/loops on the surface.

In the CR2-C3d complex, no continuous stretch of residues on C3d participates in the interactions. Rather, residues that are separated in the linear sequence of C3d, but come together on the folded C3d, interact with CR2. Namely, the residues on the H3-H4 loop (the loop between helix 3 and 4), as well as H5, and H7 make contact with CR2 (Fig. 3C). On the CR2 part, however, a linear stretch of residues within SCR2 domain makes the contact with C3d. The B strand and B-C loop of SCR2 constitute the majority of the interactions with C3d. The nature of the contacts involves elegant networks of hydrogen bonds, plus some hydrophobic and van der Waals interactions (Fig. 3D & 3E).

It is particularly intriguing that only SCR2 directly contacts C3d. Previous studies have shown that both SCR1 and SCR2 are required for binding of polymeric forms of C3d to CR2 on cell membranes (C. A. Lowell, et al., *J Exp Med* 170, 1931-46 (1989); J. C. Carel, et al., *J Biol Chem* 265, 12293-9 (1990); K. R. Kalli, et al., *J Immunol* 147, 590-4 (1991)). The requirement for both domains to bind C3d on the cell surface may be due to the necessity of inter-SCR packing for stabilization of the SCR2 site, or alternatively the dimerization of CR2 mediated by SCR1 plays a necessary role on cell membranes, as discussed later.

Specificity of CR2-C3d interaction

A few features about the CR2-C3d interactions are very striking. The first of such is the extensive use of main-chain carbonyl oxygen and nitrogen atoms in forming hydrogen bonds (H-bonds) between CR2 and C3d. This is particularly true on the C3d side, where the majority of the H-bond contributors on C3d come from main-chain carbonyl groups (Fig. 3D & 3E). No side chains other than Asn170 on the C3d side are involved in the direct interaction with CR2. This observation likely explains the difficulties in previous efforts to

accurately identify the residues that directly interact with CR2 by site-directed mutagenesis of C3d or by using C3d-derived inhibitory peptides. This interaction mode of CR2-C3d is reminiscent of MHC-antigen peptide recognition where MHC interacts with the main-chain atoms of the antigen peptide in order to allow the limited number of MHC to bind the unlimited variations of antigens for antigen presentation to T cells (P. J. Bjorkman, et al., *Nature* 329, 512-8 (1987)). However, in distinct contrast to the MHC-antigen peptide interaction, the binding between CR2 and C3d through main-chain atoms here does not sacrifice the specificity of the CR2 receptor for C3d ligand due to an additional pronounced shape-fitting requirement, as further evident in later discussion.

Another important feature concerns one of the major sites for binding CR2 on C3d at the C-terminal end of H5. Here four carbonyl groups, one each from Ile1155, Leu1166, Glu1177 and Gln1199 of C3d, are positioned in such a way that, collectively, they form an anion hole at the C-terminus of H5 (Fig. 3D). In the complex structure, this anion hole is occupied by the positively charged Arg84 of CR2 that is located on the B-C loop of SCR2 domain. In this case, CR2 Arg84 acts as a capping residue in-trans to seal the alpha-helical dipole moment at the C-terminus of H5 of C3d. This is in contrast to the usual observation in other protein-ligand interactions that involve an alpha-helical dipole moment, in which usually a negatively charged group interacts with the other protein through the positively charged N-terminus of a helix, possibly because of the easily accessible nitrogen atoms on the main-chain (C. Branden, J. Tooze, *Introduction to Protein Structure* (Garland Publishing, ed. second edition, 1999) pp.16). However, for CR2 to interact with the negatively charged C-terminus of C3d H5 that is shielded by the particular conformation at the end of H5 and its neighboring structure, it requires CR2 to have a well-matched surface around the positively charged capping residue, providing specificity to the interaction. The sequences and conformation of SCR2 around Arg84 of CR2 provides such a surface that is well-matched with the complimentary part on C3d, and that provides the necessary specificity for the interaction with C3d.

The conformation of the C3d-binding region, the B-C loop of SCR2 domain on CR2, is thus also important for the specific binding of C3d (Figs. 3C, 3D, 3E). As one means to accomplish this conformation, the B-C loop is held and presented on the surface of CR2 by strand B and C of SCR2 in such a way that Arg84 readily fits into the anion hole at the end of the C3d H5. The residue after Arg84 is Gly85, which does not have a side chain that would interfere with the CR2 and C3d interface interaction. The side chain of Ser86 forms an H-bond with a carbonyl oxygen from the H3-H4 loop of C3d through a water molecule (Fig. 3E). Other residues around Arg84 have side chains pointing away from the interface and use either their main-chain carbonyl oxygen or nitrogen atoms to form H-bonds with C3d. This mode of interaction from the CR2 side predicts that the basic capping residue Arg84, as well as Ser86, are likely the most important residues on this interaction surface, as long as they are presented in a correct conformation.

In this regard, of importance also is a sequence comparison between human CR2 and mouse CR2 (mCR2), both of which bind C3d with similar affinity (D. R. Martin et al., *J Exp Med* 174, 1299-311 (1991); J. D. Fingeroth et al., *Proc Natl Acad Sci U S A* 86, 242-6 (1989)). The SCR1-2 region of human CR2 is represented herein as SEQ ID NO:4 and is compared to the corresponding SCR1-2 region of mouse CR2 (SEQ ID NO:6). At the C3d-interacting interface the B-C loop of mCR2 SCR2 has a basic residue Lys in place of Arg84, while Gly85 and Ser86 are conserved (positions given relative to SEQ ID NO:4). Five other amino acids around Arg84 on the B-C loop are not highly conserved (Fig. 3F). The complex structure reveals, however, that the side chains of these five non-conserved residues do not participate in the CR2-C3d interaction. Importantly, Lys84 in mouse (SEQ ID NO:6) could replace Arg84 (SEQ ID NO:4) as the trans-capping residue for H5. Of interest, outside of the 5 amino acids around Lys84 (SEQ ID NO:6), there are stretches of amino acids that are the most highly conserved between human CR2 and mCR2 (Fig. 2E). These highly conserved segments likely play an important role in presenting the B-C loop in a correct conformation for specific C3d binding to mCR2.

Another feature of the complex structure is the participation of several water molecules in the interaction (Figs. 3D & 3E). Well-ordered water molecules participate in the formation of some H-bonds between CR2 and C3d, acting as water "glue" between the two proteins. Extensive participation of water molecules in mediating receptor-ligand binding is also seen in the interaction between CAR receptor (coxsacki-adenovirus receptor) and adenovirus knob protein (M. C. Bewley et al., *Science* 286, 1579-83 (1999)).

A six-coordinated Zn atom is present on the edge of the interface between CR2 and C3d (Fig. 3D). Glu117 of C3d is the only amino acid side chain that participates in the coordination. The other four coordinates are mediated by water molecules, through which H-bond connections are formed with CR2 main-chain. The contribution of the Zn coordination to the CR2-C3d binding is likely to be insignificant, because no obvious change in formation of the CR2-C3d complex can be detected in buffers with/without Zn ion, or when using a C3d mutant containing a Glu117 to Ala mutation (see next section). In addition, the binding of CR2 with C3d does not demonstrate a known cation dependence.

Example 2

The following example describes the construction of C3d mutants that affect CR2 binding.

Based on the complex structure, mutagenesis of C3d around the interface to disrupt CR2 binding was predicted to be difficult. This is because the interaction between CR2 and C3d involves mostly main-chain H-bonding, and the side chain residues play relatively small roles in the binding. However, to confirm the accuracy of the CR2-C3d interaction seen in this co-crystal structure, two informative C3d mutants were constructed. In mutant 170 (mt170; SEQ ID NO:8), residue Asn170 was changed to Arg. Asn170 is located on H7 of C3d and is the only residue on C3d that more or less points directly toward CR2 in the interface (Fig. 3E). Asn170 also packs directly with Tyr81 of CR2 as well as forms an H-bond with CR2 (Lys100) through a water molecule (Fig. 3E). In solution, this mutant protein

behaved very similarly like the wild type C3d and showed the same apparent molecular weight as the wild type in gel-filtration chromatography, suggesting correct folding. In the binding experiment assayed by native gel shift, however, the interaction between mt170 protein and CR2 was clearly less strong comparing with that between wild type C3d and CR2 (Fig. 4A, lanes 1-4 versus 9-12).

Briefly, Figs 4A and 4B show a native gel shift assay of the binding between CR2 and C3d wild type (wt) or mutants (mt). Fig. 4A shows a 6% native polyacrylamide gel of C3d alone (lanes 1, 5, and 9) or C3d plus increasing amount of CR2 (other lanes). mt170 C3d alone (lane 9) migrated slower than both wt (lane 1) and mt115 due to the introduction of a positively charged Arg residue at N170 (lane 5). CR2 alone does not enter the gel in this system. The C3d band will be shifted to the upper part of the gel when it forms a complex with CR2. The C3d concentration (for both wt and mt) is the same throughout lanes 1-12. The CR2 added to each corresponding lanes for wt and mt C3d was also the same, e.g. same amount of CR2 was added to the C3d samples in lane 2, 6 and 10, or in lanes 4, 8 and 12. In the lanes with the highest CR2 concentration (lanes 4, 8, 12), the bands of C3d wt and mt115 were completely shifted to the complex form (lane 4, 8), while mt170 (migrated slower than the wt or mt115) still contains an obvious C3d band (lane 12). These results indicate that the interaction between mt170 and CR2 is weaker than that between the wt or mt115 with CR2. The same conclusion can be drawn by comparing the intensity of the bands of the complexes containing the wt, mt115 and mt170. Fig. 4B is a graphical representation showing the intensity changes of the complex bands (measured by densitometry) as CR2 concentration increases from lanes 2 to 4 (wt), or lanes 6 to 8 (mt115), or lanes 10 to 12 (mt170). The result clearly shows that mt170 has less apparent affinity for CR2 than wt and mt115.

The result shown in this experiment is consistent with that predicted by the interaction interface seen in the complex structure. In another mutant of C3d (mt115), although three residues: Gln105, Leu116 and Glu117, were mutated to Ala, the mutant

protein has no obvious effect on CR2 binding (Fig. 4A, lanes 1-4 versus 5-8). This is consistent with the complex structure in that all these three residues, even though located within the interface area, have their side chains pointing sideways and are not involved in the direct contact with CR2. The side chain of Glu117, however, participates in the Zn coordination. This mutant showed that Zn coordination by Glu117 does not contribute significantly to CR2-C3d binding. The coordinated Zn in the structure, therefore, could simply come from the crystallization buffer which contained ZnAcetate.

Fig. 4C demonstrates the results of a competitive ELISA analysis using informative C3d mutants. In this analysis, C3d mutant Gln105Ala, Leu116Ala, Glu117Ala (designated mt115 in Figs. 4A and 4B and mut1 in Fig. 4C) manifests an equal ability as wild type C3d to block the binding of soluble full length CR2 to plate-bound wild type C3d. Therefore, mutations of these two residues which utilize only the main-chain atoms to interact with CR2 did not have an effect, which is predicted by the X-ray structure. Two other informative mutants, one Asn170Arg (designated mt170 in Figs. 4A and 4B and mut2 in Fig. 4C, also represented herein as SEQ ID NO:8) and the other a new mutant Asn170Ala, Ile115Arg, Leu116Arg (designated mut4 in Fig. 4C, also represented herein as SEQ ID NO:9), are both unable to effectively block soluble CR2 binding to plate-bound wild type C3d. Therefore, we conclude that two mutations of C3d involving Asn170, whose side-chain interacts with CR2 directly, result in substantially decreased binding to CR2.

Of interest, the mode of interaction seen here is very different from that previously predicted by C3d mutants and C3d-derived peptides (J. D. Lambris et al., *Proc Natl Acad Sci U S A* 82, 4235-9 (1985); R. J. Diefenbach et al., *J Immunol* 154, 2303-20 (1995); L. Clemenza et al., *J Immunol* 165, 3839-48 (2000)). Close examination of the complex structure, however, can explain some of the previous mutagenesis results. For example, residues Asp163, Ile164, and Glu166 of C3d, which affect CR2-binding after being mutated to Ala (Clemenza et al., 2000, *ibid.*), are located on H6 that is juxtaposed to H5 where the major CR2-recognizing anion hole is positioned (Fig. 3D). Based on the structure, it is

obvious that mutations of some of the residues on H6 (such as Ile164) of C3d will affect the relative positions of H6 and H5, which may account for the reduced interaction with CR2. The other group of mutations on C3d (Asp36, Glu37, Glu39) reported to weaken CR2 binding (Clemenza et al., 2000, *ibid.*) are located right next to the N and C termini, and the present inventors' findings cannot account for those results. However, it is of note that this particular site would be juxtaposed to additional large peptides derived from iC3b, and these additional peptides in iC3b would present a steric hindrance for the interaction with CR2 if these residues were to be involved in CR2 binding. The present inventors' observation that CR2 contacts C3d on the opposite side from the N and C termini removes that concern and is more consistent with the observed high affinity binding of CR2 to iC3b.

Example 3

The following example describes the inhibition of CR2-C3d interaction by CR2-derived peptides.

Based on the structure of the CR2-C3d complex, the results from previously reported CR2 peptide inhibition and monoclonal antibody assays can now be explained. In the peptide inhibition tests using short synthetic peptides covering all of CR2 SCR1 and SCR2, peptides from two regions were shown to inhibit CR2-C3 binding (H. Molina, et al., *J Immunol* 154, 5426-35 (1995)). One of them contains sequences that are located right on the interaction interface of CR2 seen in the complex structure, namely the sequences from the B strand and B-C loop of SCR2 (Figs. 3D & 3E). This independent result strongly supports the complex structure described by the present invention. However, the other peptide located on the B strand of SCR1 also showed a similar inhibition effect as the first one. Close examination of this fragment on CR2 structure within the SCR1 domain revealed a very similar 3-dimensional arrangement of these residues as the one on SCR2, but the sequence is in part reversed. Part of the C3d-binding sequences on the SCR2 B-C loop is 83-IRGSTP-88. The peptide from SCR1 that also has inhibitory effects has a sequence of 11-LNGRIS-16

(H. Molina et al., 1995, *ibid*). Similarities are apparent between these two peptides if one of the sequences is reversed. Specifically, at the 3-dimensional structure level, the conformation of -NGRI- of the SCR1 peptide looks like a reverse duplicate of -IRGS- on SCR2. However, in a folded CR2 molecule, the structure of the neighboring residues around the peptide on SCR1 restricts the accessibility of the sequences within the peptide, especially the Arg residue. Therefore, this part of CR2 should not be able to bind C3d unless some major conformational switch occurred to expose the segment in a fashion similar to it in a short peptide state.

Example 4

The following example describes the inhibition of CR2-C3d binding by anti-CR2 monoclonal antibodies.

The previously mapped epitope positions on CR2 for inhibitory monoclonal antibodies also support the interaction sites seen in the CR2-C3d complex structure. Two inhibitory antibodies, OKB7 (P. E. Rao et al., *Cell Immunol* 93, 549-55 (1985)) and FE8 (W. M. Prodinger, et al., *J Immunol* 161, 4604-10 (1998)), have epitopes positioned right next to the C3d binding region (Figs. 5A & 5B). The present inventors have also created three new monoclonal antibodies, denoted mAb171, mAb1048 and mAb629, that inhibit the specific binding of CR2 to C3d. All three have mapped epitopes on CR2 lying right within the C3d-interacting area (Fig. 5A, blue area).

Figs. 5A and 5B show the localization of the epitopes of anti-CR2 monoclonal antibodies (mAb) on the CR2 surface. These figures are two views with a 180 degree rotation to each other. The C3d binding site is labeled. All of the mAbs inhibit the interactions between CR2 and C3d to some extent. mAb171, together with 1048 and 629 (colored in blue) have epitopes located within the C3d-binding area. OKB7 (Rao et al., 1985, *ibid.*) (colored in red) and FE8 (Prodinger et al., 1998, *ibid.*) (colored in pink) also have epitopes right next to the C3d-binding region. The green spots indicate the locations

where mutations from mCR2 to hCR2 sequence allow mCR2 to gain the ability to bind EBV gp350/220. The surfaces around these two sites are likely located within the interface between CR2 and gp350/220.

Example 5

The following example describes a potential gp350/220 binding region in CR2.

Previous evidence suggests that CR2 binds to C3d and EBV gp350/220 with overlapping but distinct sites (D. R. Martin et al., *J Exp Med* 174, 1299-311 (1991); H. Molina et al., *J Biol Chem* 266, 12173-9 (1991); D. R. Martin et al., *J Virol* 68, 4716-26 (1994); H. Molina et al., *J Immunol* 154, 5426-35 (1995)). One instrumental result in this regard has been the ability to transform by point mutation mCR2 into a form capable of binding gp350/220. In this regard, mCR2 and CR2 both bind C3d, but mCR2 does not bind EBV or gp350/220. However, changing the sequence of mCR2 at two amino acids (Pro16 to Ser and Thr69 to Tyr, Fig. 2E) allowed mCR2 to gain the ability to bind EBV (D. R. Martin et al., *J Virol* 68, 4716-26 (1994)). Because of this, the locations of the two mutated residues are likely to be involved in gp350/220 binding. Of interest, these locations mapped on the CR2 surface (green patch on Figs. 5A & 5B) are separated from the blue area that interacts with C3d in the complex structure of the present invention.

Example 6

The following example describes a structure model of CR2 in complex with C3d on the cell surface.

Based on the complex structure, the present inventors propose a model of CR2 binding to C3d or iC3b on the cell surface (Fig. 6). Fig. 6A is a surface representation of the model containing a dimer of CR2 SCR1 and SCR2 that bind to C3d on each receptor. The dimer contact is through SCR1 only, as seen in the crystal structure. Fig. 6B is a diagram of C3d-antigen cross-linking CR2 (as dimers) and BCR on the cell surface. The dimer form of

CR2, as opposed to the monomer, in complex with CD19/CD81 permits the cross-linking of multiple CR2 by C3d-antigen to greatly increase the local concentration of CR2/CD19/CD81.

In this model, CR2 in complex with C3d molecules exists as a dimer through SCR1-SCR1 contact (Figs. 6A & 6B). C3d- or iC3b-bound antigen interacts with SCR2 in such a way that the site of ester-linkage with the antigen (residue Q20) is pointing in the lateral direction (Fig. 6A). This orientation allows CR2 maximum capabilities to interact with C3 bound to many shapes and sizes of antigens. In addition, though, there is also the opportunity for the antigen to cross-link a neighboring CR2 dimer with a second C3d/iC3b attached to it. Repeat of this interaction could cross-link many CR2/CD19/CD81and BCR molecules, with the potential of greatly amplifying down-stream signal transduction. Of interest, previous reports of C3d acting as a molecular adjuvant showed that two or three C3d attached to hen egg lysozyme (HEL) enhanced the IgG1 humoral response to HEL by 1,000 to 10,000 times, but one C3d had a suppressive effect (P. W. Dempsey et al., *Science* 271, 348-50 (1996)). The model in Fig. 6B provides one potential molecular explanation for this observation. Multiple CR2 dimers can be brought together by two (or more) C3d linked to an antigen, but only two (or three) CR2 monomers can be cross-linked together. Thus, the CR2 dimer model, in contrast to a monomer, allows a dramatic increase of cross-linked CR2/CD19/CD81 and BCR molecules through binding to the antigen with two or more C3d attached, which could account for the 10,000-fold enhancement of the observed immune response.

TABLE 2

ATOM	1	CB	ALA	A	1	113.978	74.531	51.463	1.00	24.47	A
ATOM	2	C	ALA	A	1	113.746	72.085	52.035	1.00	26.48	A
ATOM	3	O	ALA	A	1	112.896	72.106	52.942	1.00	30.12	A
ATOM	4	N	ALA	A	1	115.853	72.884	51.119	1.00	42.70	A
ATOM	5	CA	ALA	A	1	114.718	73.256	51.995	1.00	33.68	A
ATOM	6	N	LEU	A	2	113.868	71.065	52.232	1.00	24.18	A
ATOM	7	CA	LEU	A	2	112.952	69.905	51.320	1.00	27.55	A
ATOM	8	CB	LEU	A	2	112.148	69.728	50.001	1.00	23.79	A
ATOM	9	CG	LEU	A	2	110.907	68.774	50.002	1.00	26.21	A
ATOM	10	CD1	LEU	A	2	109.785	69.339	50.877	1.00	20.38	A
ATOM	11	CD2	LEU	A	2	110.365	68.568	48.962	1.00	22.09	A
ATOM	12	C	LEU	A	2	113.635	68.549	51.642	1.00	27.27	A
ATOM	13	O	LEU	A	2	114.746	68.266	51.172	1.00	22.30	A
ATOM	14	N	ASP	A	3	112.963	67.734	52.455	1.00	23.38	A
ATOM	15	CA	ASP	A	3	113.426	66.393	52.758	1.00	23.91	A
ATOM	16	CB	ASP	A	3	114.304	65.827	54.028	1.00	20.20	A
ATOM	17	CG	ASP	A	3	113.619	66.825	55.279	1.00	22.03	A
ATOM	18	OD1	ASP	A	3	112.357	66.765	55.433	1.00	20.42	A
ATOM	19	OD2	ASP	A	3	114.366	67.274	56.160	1.00	28.30	A
ATOM	20	C	ASP	A	3	112.201	65.488	52.875	1.00	23.39	A
ATOM	21	O	ASP	A	3	111.047	65.963	52.784	1.00	18.32	A
ATOM	22	N	ALA	A	4	112.438	64.194	53.060	1.00	24.33	A
ATOM	23	CA	ALA	A	4	111.330	63.243	53.164	1.00	23.20	A
ATOM	24	CB	ALA	A	4	111.854	61.819	53.088	1.00	17.28	A
ATOM	25	C	ALA	A	4	110.291	63.499	54.261	1.00	19.39	A
ATOM	26	O	ALA	A	4	109.113	63.359	53.958	1.00	16.69	A
ATOM	27	N	GLU	A	5	110.691	63.841	55.491	1.00	16.50	A
ATOM	28	CA	GLU	A	5	109.701	64.065	56.548	1.00	22.14	A
ATOM	29	CB	GLU	A	5	110.301	64.257	57.982	1.00	23.56	A
ATOM	30	CG	GLU	A	5	110.935	65.596	58.262	1.00	38.23	A
ATOM	31	CD	GLU	A	5	110.138	66.605	59.095	1.00	31.60	A
ATOM	32	OE1	GLU	A	5	109.004	66.387	59.598	1.00	31.04	A
ATOM	33	OE2	GLU	A	5	110.719	67.671	59.253	1.00	44.56	A
ATOM	34	C	GLU	A	5	108.853	65.280	56.208	1.00	20.89	A
ATOM	35	O	GLU	A	5	107.637	65.242	56.419	1.00	22.09	A
ATOM	36	N	ARG	A	6	109.470	66.309	55.662	1.00	17.73	A
ATOM	37	CA	ARG	A	6	108.703	67.491	55.302	1.00	23.39	A
ATOM	38	CB	ARG	A	6	109.618	68.614	54.815	1.00	25.00	A
ATOM	39	CG	ARG	A	6	110.433	69.134	55.948	1.00	24.66	A
ATOM	40	CD	ARG	A	6	111.430	70.240	55.488	1.00	30.21	A
ATOM	41	NE	ARG	A	6	112.143	70.710	56.662	1.00	31.75	A
ATOM	42	CZ	ARG	A	6	113.044	71.686	56.675	1.00	37.88	A
ATOM	43	NH1	ARG	A	6	113.377	72.353	55.558	1.00	32.11	A
ATOM	44	NH2	ARG	A	6	113.608	72.015	57.830	1.00	38.98	A
ATOM	45	C	ARG	A	6	107.696	67.156	54.219	1.00	25.83	A
ATOM	46	O	ARG	A	6	106.532	67.558	54.304	1.00	20.78	A
ATOM	47	N	LEU	A	7	108.122	66.404	53.205	1.00	19.12	A
ATOM	48	CA	LEU	A	7	107.179	65.963	52.145	1.00	17.13	A
ATOM	49	CB	LEU	A	7	107.916	65.488	50.945	1.00	16.82	A
ATOM	50	CG	LEU	A	7	106.984	65.041	49.805	1.00	23.63	A
ATOM	51	CD1	LEU	A	7	106.086	66.207	49.303	1.00	18.87	A
ATOM	52	CD2	LEU	A	7	107.870	64.538	48.676	1.00	25.78	A
ATOM	53	C	LEU	A	7	106.103	65.075	52.615	1.00	19.67	A

ATOM	54	O	LEU	A	7	104.935	65.191	52.246	1.00	20.24	A
ATOM	55	N	LYS	A	8	106.489	64.099	53.427	1.00	21.02	A
ATOM	56	CA	LYS	A	8	105.521	63.110	53.928	1.00	24.15	A
ATOM	57	CB	LYS	A	8	106.205	62.100	54.859	1.00	26.98	A
ATOM	58	CG	LYS	A	8	105.339	60.838	55.146	1.00	29.12	A
ATOM	59	CD	LYS	A	8	105.997	59.844	56.108	1.00	48.06	A
ATOM	60	CE	LYS	A	8	107.390	59.397	55.608	1.00	61.21	A
ATOM	61	NZ	LYS	A	8	108.117	58.353	56.469	1.00	69.61	A
ATOM	62	C	LYS	A	8	104.281	63.720	54.630	1.00	22.77	A
ATOM	63	O	LYS	A	8	103.163	63.203	54.499	1.00	16.94	A
ATOM	64	N	HIS	A	9	104.465	64.778	55.412	1.00	17.13	A
ATOM	65	CA	HIS	A	9	103.303	65.454	56.034	1.00	23.94	A
ATOM	66	CB	HIS	A	9	103.759	66.675	56.838	1.00	15.51	A
ATOM	67	CG	HIS	A	9	104.457	66.331	58.109	1.00	25.05	A
ATOM	68	CD2	HIS	A	9	105.755	66.445	58.478	1.00	22.49	A
ATOM	69	ND1	HIS	A	9	103.792	65.831	59.209	1.00	24.32	A
ATOM	70	CE1	HIS	A	9	104.649	65.654	60.200	1.00	26.37	A
ATOM	71	NE2	HIS	A	9	105.851	66.015	59.786	1.00	31.51	A
ATOM	72	C	HIS	A	9	102.268	65.959	55.002	1.00	24.84	A
ATOM	73	O	HIS	A	9	101.161	66.278	55.375	1.00	23.11	A
ATOM	74	N	LEU	A	10	102.634	66.074	53.721	1.00	18.19	A
ATOM	75	CA	LEU	A	10	101.670	66.538	52.730	1.00	22.98	A
ATOM	76	CB	LEU	A	10	102.370	67.210	51.534	1.00	24.09	A
ATOM	77	CG	LEU	A	10	103.171	68.492	51.885	1.00	30.55	A
ATOM	78	CD1	LEU	A	10	103.625	69.205	50.648	1.00	29.82	A
ATOM	79	CD2	LEU	A	10	102.285	69.415	52.701	1.00	39.35	A
ATOM	80	C	LEU	A	10	100.789	65.391	52.237	1.00	30.17	A
ATOM	81	O	LEU	A	10	99.875	65.616	51.442	1.00	31.15	A
ATOM	82	N	ILE	A	11	101.065	64.159	52.663	1.00	20.98	A
ATOM	83	CA	ILE	A	11	100.194	63.053	52.229	1.00	22.19	A
ATOM	84	CB	ILE	A	11	101.002	61.747	52.060	1.00	27.01	A
ATOM	85	CG2	ILE	A	11	100.044	60.547	51.788	1.00	29.34	A
ATOM	86	CG1	ILE	A	11	101.984	61.940	50.863	1.00	21.97	A
ATOM	87	CD1	ILE	A	11	103.039	60.904	50.736	1.00	31.22	A
ATOM	88	C	ILE	A	11	99.082	62.956	53.269	1.00	27.58	A
ATOM	89	O	ILE	A	11	99.300	62.542	54.411	1.00	26.44	A
ATOM	90	N	VAL	A	12	97.890	63.403	52.888	1.00	23.12	A
ATOM	91	CA	VAL	A	12	96.760	63.400	53.803	1.00	22.74	A
ATOM	92	CB	VAL	A	12	96.392	64.814	54.185	1.00	33.31	A
ATOM	93	CG1	VAL	A	12	97.530	65.452	55.004	1.00	34.31	A
ATOM	94	CG2	VAL	A	12	96.105	65.600	52.928	1.00	24.64	A
ATOM	95	C	VAL	A	12	95.487	62.726	53.265	1.00	28.78	A
ATOM	96	O	VAL	A	12	95.316	62.525	52.061	1.00	25.51	A
ATOM	97	N	THR	A	13	94.577	62.396	54.174	1.00	22.73	A
ATOM	98	CA	THR	A	13	93.348	61.747	53.787	1.00	24.33	A
ATOM	99	CB	THR	A	13	92.824	60.803	54.947	1.00	28.46	A
ATOM	100	OG1	THR	A	13	93.834	59.921	55.298	1.00	37.06	A
ATOM	101	CG2	THR	A	13	91.503	60.186	54.540	1.00	22.36	A
ATOM	102	C	THR	A	13	92.328	62.811	53.443	1.00	19.70	A
ATOM	103	O	THR	A	13	92.043	63.649	54.254	1.00	18.28	A
ATOM	104	N	PRO	A	14	91.760	62.781	52.239	1.00	23.16	A
ATOM	105	CD	PRO	A	14	92.057	61.889	51.100	1.00	27.40	A
ATOM	106	CA	PRO	A	14	90.765	63.803	51.883	1.00	23.69	A
ATOM	107	CB	PRO	A	14	90.675	63.699	50.355	1.00	20.22	A
ATOM	108	CG	PRO	A	14	90.959	62.232	50.106	1.00	26.75	A

ATOM	109	C	PRO	A	14	89.406	63.564	52.509	1.00	22.95	A
ATOM	110	O	PRO	A	14	89.009	62.415	52.725	1.00	20.64	A
ATOM	111	N	SER	A	15	88.719	64.651	52.845	1.00	19.26	A
ATOM	112	CA	SER	A	15	87.348	64.575	53.337	1.00	25.94	A
ATOM	113	CB	SER	A	15	87.295	64.124	54.797	1.00	25.47	A
ATOM	114	OG	SER	A	15	88.078	64.979	55.578	1.00	28.02	A
ATOM	115	C	SER	A	15	86.638	65.928	53.187	1.00	26.13	A
ATOM	116	O	SER	A	15	87.227	66.923	52.758	1.00	26.66	A
ATOM	117	N	GLY	A	16	85.364	65.948	53.556	1.00	28.55	A
ATOM	118	CA	GLY	A	16	84.593	67.167	53.481	1.00	25.28	A
ATOM	119	C	GLY	A	16	83.748	67.259	52.225	1.00	23.22	A
ATOM	120	O	GLY	A	16	83.667	66.314	51.428	1.00	20.49	A
ATOM	121	N	ALA	A	17	83.122	68.421	52.072	1.00	21.03	A
ATOM	122	CA	ALA	A	17	82.258	68.742	50.952	1.00	19.04	A
ATOM	123	CB	ALA	A	17	81.288	69.898	51.356	1.00	17.25	A
ATOM	124	C	ALA	A	17	83.051	69.097	49.692	1.00	19.33	A
ATOM	125	O	ALA	A	17	84.271	68.928	49.643	1.00	22.08	A
ATOM	126	N	GLY	A	18	82.356	69.566	48.668	1.00	17.15	A
ATOM	127	CA	GLY	A	18	82.983	69.869	47.376	1.00	17.27	A
ATOM	128	C	GLY	A	18	84.233	70.743	47.300	1.00	21.54	A
ATOM	129	O	GLY	A	18	84.993	70.629	46.350	1.00	16.56	A
ATOM	130	N	GLU	A	19	84.419	71.653	48.248	1.00	18.40	A
ATOM	131	CA	GLU	A	19	85.629	72.488	48.258	1.00	22.07	A
ATOM	132	CB	GLU	A	19	85.302	73.929	48.683	1.00	14.92	A
ATOM	133	CG	GLU	A	19	84.450	74.722	47.650	1.00	18.57	A
ATOM	134	CD	GLU	A	19	84.034	76.086	48.184	1.00	21.03	A
ATOM	135	OE1	GLU	A	19	84.654	76.565	49.162	1.00	20.93	A
ATOM	136	OE2	GLU	A	19	83.096	76.694	47.639	1.00	19.11	A
ATOM	137	C	GLU	A	19	86.679	71.889	49.203	1.00	18.24	A
ATOM	138	O	GLU	A	19	87.865	71.779	48.822	1.00	17.08	A
ATOM	139	N	GLN	A	20	86.235	71.519	50.415	1.00	15.20	A
ATOM	140	CA	GLN	A	20	87.084	70.923	51.502	1.00	20.25	A
ATOM	141	CB	GLN	A	20	86.217	70.526	52.751	1.00	23.39	A
ATOM	142	CG	GLN	A	20	85.294	71.692	53.342	1.00	43.73	A
ATOM	143	CD	GLN	A	20	84.079	71.273	54.096	1.00	42.02	A
ATOM	144	OE1	GLN	A	20	83.301	70.366	53.989	1.00	38.04	A
ATOM	145	NE2	GLN	A	20	83.924	71.988	55.410	1.00	35.68	A
ATOM	146	C	GLN	A	20	87.816	69.660	50.976	1.00	24.37	A
ATOM	147	O	GLN	A	20	88.996	69.451	51.237	1.00	17.93	A
ATOM	148	N	ASN	A	21	87.100	68.832	50.225	1.00	15.50	A
ATOM	149	CA	ASN	A	21	87.677	67.616	49.677	1.00	18.10	A
ATOM	150	CB	ASN	A	21	86.601	66.790	48.967	1.00	13.23	A
ATOM	151	CG	ASN	A	21	87.145	65.457	48.485	1.00	23.30	A
ATOM	152	OD1	ASN	A	21	87.490	64.598	49.294	1.00	17.88	A
ATOM	153	ND2	ASN	A	21	87.251	65.294	47.168	1.00	17.11	A
ATOM	154	C	ASN	A	21	88.047	67.895	48.721	1.00	21.18	A
ATOM	155	O	ASN	A	21	89.789	67.088	48.658	1.00	21.46	A
ATOM	156	N	MET	A	22	88.787	69.004	47.971	1.00	14.28	A
ATOM	157	CA	MET	A	22	89.850	69.360	47.039	1.00	12.72	A
ATOM	158	CB	MET	A	22	89.330	70.305	45.939	1.00	19.05	A
ATOM	159	CG	MET	A	22	88.285	69.647	45.064	1.00	20.17	A
ATOM	160	SD	MET	A	22	88.876	68.159	44.293	1.00	28.53	A
ATOM	161	CE	MET	A	22	90.211	68.915	43.271	1.00	21.96	A
ATOM	162	C	MET	A	22	91.028	69.995	47.767	1.00	15.63	A
ATOM	163	O	MET	A	22	92.159	69.896	47.328	1.00	16.97	A

ATOM	164	N	ILE	A	23	90.743	70.644	48.886	1.00	11.88	A
ATOM	165	CA	ILE	A	23	91.784	71.242	49.714	1.00	19.19	A
ATOM	166	CB	ILE	A	23	91.126	72.029	50.870	1.00	13.50	A
ATOM	167	CG2	ILE	A	23	92.159	72.357	51.971	1.00	13.80	A
ATOM	168	CG1	ILE	A	23	90.476	73.296	50.297	1.00	16.98	A
ATOM	169	CD1	ILE	A	23	89.807	74.203	51.351	1.00	17.93	A
ATOM	170	C	ILE	A	23	92.597	70.046	50.235	1.00	22.66	A
ATOM	171	O	ILE	A	23	93.843	70.053	50.257	1.00	18.47	A
ATOM	172	N	GLY	A	24	91.892	68.990	50.628	1.00	15.67	A
ATOM	173	CA	GLY	A	24	92.583	67.804	51.110	1.00	17.85	A
ATOM	174	C	GLY	A	24	93.291	67.056	50.000	1.00	21.53	A
ATOM	175	O	GLY	A	24	94.439	66.616	50.138	1.00	16.68	A
ATOM	176	N	MET	A	25	92.631	66.918	48.864	1.00	18.50	A
ATOM	177	CA	MET	A	25	93.234	66.170	47.767	1.00	15.73	A
ATOM	178	CB	MET	A	25	92.153	65.985	46.703	1.00	21.35	A
ATOM	179	CG	MET	A	25	92.469	65.151	45.529	1.00	26.92	A
ATOM	180	SD	MET	A	25	90.966	64.905	44.498	1.00	24.37	A
ATOM	181	CE	MET	A	25	91.718	63.617	43.360	1.00	17.81	A
ATOM	182	C	MET	A	25	94.511	66.832	47.185	1.00	23.64	A
ATOM	183	O	MET	A	25	95.432	66.146	46.757	1.00	17.81	A
ATOM	184	N	THR	A	26	94.577	68.164	47.180	1.00	17.90	A
ATOM	185	CA	THR	A	26	95.736	68.856	46.607	1.00	18.87	A
ATOM	186	CB	THR	A	26	95.629	70.395	46.847	1.00	17.83	A
ATOM	187	OG1	THR	A	26	94.436	70.869	46.218	1.00	17.41	A
ATOM	188	CG2	THR	A	26	96.851	71.139	46.262	1.00	16.75	A
ATOM	189	C	THR	A	26	97.149	68.423	47.052	1.00	11.10	A
ATOM	190	O	THR	A	26	97.990	68.069	46.229	1.00	17.69	A
ATOM	191	N	PRO	A	27	97.418	68.448	48.353	1.00	13.60	A
ATOM	192	CD	PRO	A	27	96.664	68.937	49.532	1.00	11.14	A
ATOM	193	CA	PRO	A	27	98.788	68.049	48.696	1.00	17.00	A
ATOM	194	CB	PRO	A	27	98.861	68.267	50.218	1.00	12.53	A
ATOM	195	CG	PRO	A	27	97.406	68.312	50.676	1.00	15.76	A
ATOM	196	C	PRO	A	27	99.193	66.662	48.277	1.00	21.64	A
ATOM	197	O	PRO	A	27	100.304	66.455	47.840	1.00	19.29	A
ATOM	198	N	THR	A	28	98.273	65.709	48.393	1.00	16.44	A
ATOM	199	CA	THR	A	28	98.607	64.333	48.046	1.00	17.14	A
ATOM	200	CB	THR	A	28	97.488	63.396	48.522	1.00	13.78	A
ATOM	201	OG1	THR	A	28	97.290	63.620	49.926	1.00	16.04	A
ATOM	202	CG2	THR	A	28	97.822	61.967	48.263	1.00	20.93	A
ATOM	203	C	THR	A	28	98.827	64.211	46.567	1.00	19.51	A
ATOM	204	O	THR	A	28	99.799	63.572	46.116	1.00	17.24	A
ATOM	205	N	VAL	A	29	97.957	64.844	45.781	1.00	16.43	A
ATOM	206	CA	VAL	A	29	98.164	64.762	44.346	1.00	16.98	A
ATOM	207	CB	VAL	A	29	97.035	65.430	43.524	1.00	21.71	A
ATOM	208	CG1	VAL	A	29	97.421	65.427	41.999	1.00	14.09	A
ATOM	209	CG2	VAL	A	29	95.731	64.619	43.708	1.00	22.05	A
ATOM	210	C	VAL	A	29	99.474	65.393	43.939	1.00	24.43	A
ATOM	211	O	VAL	A	29	100.260	64.768	43.179	1.00	19.52	A
ATOM	212	N	ILE	A	30	99.767	66.608	44.420	1.00	21.18	A
ATOM	213	CA	ILE	A	30	101.022	67.194	43.950	1.00	21.90	A
ATOM	214	CB	ILE	A	30	101.165	68.700	44.228	1.00	25.58	A
ATOM	215	CG2	ILE	A	30	100.124	69.422	43.519	1.00	45.44	A
ATOM	216	CG1	ILE	A	30	101.109	68.995	45.713	1.00	20.88	A
ATOM	217	CD1	ILE	A	30	102.385	68.792	46.400	1.00	43.61	A
ATOM	218	C	ILE	A	30	102.227	66.495	44.510	1.00	8.84	A

ATOM	219	O	ILE	A	30	103.227	66.413	43.837	1.00	20.78	A
ATOM	220	N	ALA	A	31	102.137	65.986	45.730	1.00	11.98	A
ATOM	221	CA	ALA	A	31	103.289	65.247	46.282	1.00	16.32	A
ATOM	222	CB	ALA	A	31	102.982	64.774	47.668	1.00	11.90	A
ATOM	223	C	ALA	A	31	103.613	64.026	45.381	1.00	20.08	A
ATOM	224	O	ALA	A	31	104.779	63.774	45.047	1.00	18.22	A
ATOM	225	N	VAL	A	32	102.594	63.254	45.005	1.00	16.38	A
ATOM	226	CA	VAL	A	32	102.452	62.078	44.161	1.00	18.95	A
ATOM	227	CB	VAL	A	32	101.697	61.176	44.042	1.00	22.56	A
ATOM	228	CG1	VAL	A	32	101.803	60.122	42.937	1.00	22.34	A
ATOM	229	CG2	VAL	A	32	101.348	60.477	45.364	1.00	13.55	A
ATOM	230	C	VAL	A	32	103.328	62.569	42.778	1.00	22.75	A
ATOM	231	O	VAL	A	32	104.310	62.061	42.211	1.00	22.15	A
ATOM	232	N	HIS	A	33	102.662	63.581	42.234	1.00	17.13	A
ATOM	233	CA	HIS	A	33	103.113	64.112	40.945	1.00	15.67	A
ATOM	234	CB	HIS	A	33	102.301	65.335	40.554	1.00	19.93	A
ATOM	235	CG	HIS	A	33	102.849	66.078	39.380	1.00	19.22	A
ATOM	236	CD2	HIS	A	33	103.579	67.220	39.317	1.00	25.53	A
ATOM	237	ND1	HIS	A	33	102.541	65.747	38.076	1.00	24.42	A
ATOM	238	CE1	HIS	A	33	103.042	66.661	37.262	1.00	21.19	A
ATOM	239	NE2	HIS	A	33	103.674	67.567	37.992	1.00	27.74	A
ATOM	240	C	HIS	A	33	104.580	64.549	41.036	1.00	15.68	A
ATOM	241	O	HIS	A	33	105.354	64.348	40.108	1.00	20.03	A
ATOM	242	N	TYR	A	34	104.944	65.179	42.144	1.00	16.97	A
ATOM	243	CA	TYR	A	34	106.317	65.646	42.304	1.00	20.05	A
ATOM	244	CB	TYR	A	34	106.420	66.500	43.571	1.00	19.93	A
ATOM	245	CG	TYR	A	34	107.826	66.882	43.969	1.00	14.48	A
ATOM	246	CD1	TYR	A	34	108.374	68.143	43.629	1.00	19.63	A
ATOM	247	CE1	TYR	A	34	109.672	68.522	44.095	1.00	15.16	A
ATOM	248	CD2	TYR	A	34	108.597	66.021	44.746	1.00	21.63	A
ATOM	249	CE2	TYR	A	34	109.889	66.380	45.183	1.00	17.33	A
ATOM	250	CZ	TYR	A	34	110.419	67.633	44.861	1.00	21.32	A
ATOM	251	OH	TYR	A	34	111.695	67.974	45.318	1.00	20.25	A
ATOM	252	C	TYR	A	34	107.306	64.471	42.392	1.00	21.84	A
ATOM	253	O	TYR	A	34	108.289	64.514	41.770	1.00	20.07	A
ATOM	254	N	LEU	A	35	107.010	63.454	43.197	1.00	19.69	A
ATOM	255	CA	LEU	A	35	107.924	62.333	43.345	1.00	19.40	A
ATOM	256	CB	LEU	A	35	107.452	61.435	44.478	1.00	17.56	A
ATOM	257	CG	LEU	A	35	107.627	62.047	45.884	1.00	16.05	A
ATOM	258	CD1	LEU	A	35	106.927	61.165	46.915	1.00	19.26	A
ATOM	259	CD2	LEU	A	35	109.123	62.096	46.253	1.00	15.28	A
ATOM	260	C	LEU	A	35	108.066	61.564	42.015	1.00	23.12	A
ATOM	261	O	LEU	A	35	109.187	61.215	41.608	1.00	17.85	A
ATOM	262	N	ASP	A	36	106.954	61.305	41.329	1.00	16.70	A
ATOM	263	CA	ASP	A	36	107.009	60.614	40.024	1.00	21.87	A
ATOM	264	CB	ASP	A	36	105.720	60.458	39.375	1.00	23.42	A
ATOM	265	CG	ASP	A	36	104.722	59.442	40.071	1.00	19.96	A
ATOM	266	OD1	ASP	A	36	105.160	58.736	41.003	1.00	23.17	A
ATOM	267	OD2	ASP	A	36	103.556	59.366	39.646	1.00	26.39	A
ATOM	268	C	ASP	A	36	107.830	61.430	39.021	1.00	26.32	A
ATOM	269	O	ASP	A	36	108.760	60.927	38.360	1.00	22.51	A
ATOM	270	N	GLU	A	37	107.505	62.709	38.909	1.00	19.41	A
ATOM	271	CA	GLU	A	37	108.180	63.550	37.919	1.00	23.12	A
ATOM	272	CB	GLU	A	37	107.476	64.916	37.874	1.00	31.20	A
ATOM	273	CG	GLU	A	37	107.620	65.640	36.601	1.00	42.72	A

ATOM	274	CD	GLU	A	37	106.461	65.412	35.676	1.00	49.79	A
ATOM	275	OE1	GLU	A	37	106.263	64.269	35.210	1.00	51.12	A
ATOM	276	OE2	GLU	A	37	105.728	66.387	35.415	1.00	58.13	A
ATOM	277	C	GLU	A	37	109.679	63.735	38.197	1.00	28.37	A
ATOM	278	O	GLU	A	37	110.506	63.788	37.269	1.00	19.17	A
ATOM	279	N	THR	A	38	110.044	63.821	39.469	1.00	19.70	A
ATOM	280	CA	THR	A	38	111.446	64.046	39.777	1.00	18.16	A
ATOM	281	CB	THR	A	38	111.615	64.951	41.051	1.00	24.32	A
ATOM	282	OG1	THR	A	38	111.062	64.292	42.206	1.00	17.55	A
ATOM	283	CG2	THR	A	38	110.872	66.295	40.874	1.00	17.35	A
ATOM	284	C	THR	A	38	112.173	62.725	39.992	1.00	23.12	A
ATOM	285	O	THR	A	38	113.384	62.708	40.176	1.00	20.01	A
ATOM	286	N	GLU	A	39	111.423	61.626	39.973	1.00	19.41	A
ATOM	287	CA	GLU	A	39	111.997	60.298	40.178	1.00	24.05	A
ATOM	288	CB	GLU	A	39	112.918	59.965	38.997	1.00	26.82	A
ATOM	289	CG	GLU	A	39	112.089	59.751	37.704	1.00	27.56	A
ATOM	290	CD	GLU	A	39	112.915	59.531	36.414	1.00	40.15	A
ATOM	291	OE1	GLU	A	39	113.910	58.776	36.430	1.00	32.93	A
ATOM	292	OE2	GLU	A	39	112.555	60.113	35.358	1.00	42.52	A
ATOM	293	C	GLU	A	39	112.740	60.228	41.519	1.00	25.56	A
ATOM	294	O	GLU	A	39	113.898	59.818	41.597	1.00	23.18	A
ATOM	295	N	GLN	A	40	112.059	60.614	42.601	1.00	24.46	A
ATOM	296	CA	GLN	A	40	112.707	60.592	43.899	1.00	18.16	A
ATOM	297	CB	GLN	A	40	112.682	62.002	44.489	1.00	24.56	A
ATOM	298	CG	GLN	A	40	113.517	63.012	43.708	1.00	10.67	A
ATOM	299	CD	GLN	A	40	113.705	64.283	44.507	1.00	19.34	A
ATOM	300	OE1	GLN	A	40	114.594	64.350	45.334	1.00	17.51	A
ATOM	301	NE2	GLN	A	40	112.845	65.298	44.275	1.00	17.15	A
ATOM	302	C	GLN	A	40	112.118	59.603	44.894	1.00	19.24	A
ATOM	303	O	GLN	A	40	112.350	59.725	46.100	1.00	23.09	A
ATOM	304	N	TRP	A	41	111.345	58.635	44.403	1.00	18.32	A
ATOM	305	CA	TRP	A	41	110.700	57.670	45.311	1.00	18.31	A
ATOM	306	CB	TRP	A	41	109.808	56.715	44.511	1.00	18.08	A
ATOM	307	CG	TRP	A	41	108.504	57.334	44.147	1.00	16.18	A
ATOM	308	CD2	TRP	A	41	107.382	57.574	45.024	1.00	18.90	A
ATOM	309	CE2	TRP	A	41	106.376	58.204	44.257	1.00	16.03	A
ATOM	310	CE3	TRP	A	41	107.134	57.322	46.379	1.00	16.13	A
ATOM	311	CD1	TRP	A	41	108.139	57.816	42.926	1.00	20.37	A
ATOM	312	NE1	TRP	A	41	106.860	58.344	42.977	1.00	19.88	A
ATOM	313	CZ2	TRP	A	41	105.136	58.583	44.800	1.00	15.32	A
ATOM	314	CZ3	TRP	A	41	105.893	57.703	46.929	1.00	19.86	A
ATOM	315	CH2	TRP	A	41	104.908	58.330	46.127	1.00	17.50	A
ATOM	316	C	TRP	A	41	111.717	56.895	46.152	1.00	23.10	A
ATOM	317	O	TRP	A	41	111.457	56.555	47.312	1.00	24.58	A
ATOM	318	N	GLU	A	42	112.886	56.633	45.587	1.00	22.30	A
ATOM	319	CA	GLU	A	42	113.937	55.916	46.322	1.00	30.40	A
ATOM	320	CB	GLU	A	42	115.163	55.750	45.427	1.00	36.58	A
ATOM	321	CG	GLU	A	42	116.448	55.477	46.147	1.00	53.35	A
ATOM	322	CD	GLU	A	42	116.751	54.016	46.210	1.00	62.20	A
ATOM	323	OE1	GLU	A	42	117.946	53.652	46.164	1.00	67.07	A
ATOM	324	OE2	GLU	A	42	115.790	53.227	46.306	1.00	71.58	A
ATOM	325	C	GLU	A	42	114.292	56.689	47.595	1.00	26.77	A
ATOM	326	O	GLU	A	42	114.483	56.112	48.658	1.00	25.14	A
ATOM	327	N	LYS	A	43	114.352	58.005	47.515	1.00	24.54	A
ATOM	328	CA	LYS	A	43	114.639	58.771	48.717	1.00	25.18	A

ATOM	329	CB	LYS	A	43	115.106	60.173	48.344	1.00	33.24	A
ATOM	330	CG	LYS	A	43	116.398	60.152	47.566	1.00	36.94	A
ATOM	331	CD	LYS	A	43	117.068	61.498	47.549	1.00	39.52	A
ATOM	332	CE	LYS	A	43	116.841	62.204	46.242	1.00	39.10	A
ATOM	333	NZ	LYS	A	43	117.597	63.486	46.197	1.00	37.63	A
ATOM	334	C	LYS	A	43	113.437	58.885	49.640	1.00	30.60	A
ATOM	335	O	LYS	A	43	113.583	59.064	50.854	1.00	28.31	A
ATOM	336	N	PHE	A	44	112.232	58.754	49.089	1.00	23.22	A
ATOM	337	CA	PHE	A	44	111.061	58.940	49.924	1.00	22.11	A
ATOM	338	CB	PHE	A	44	109.995	59.654	49.078	1.00	19.24	A
ATOM	339	CG	PHE	A	44	108.732	59.989	49.809	1.00	21.27	A
ATOM	340	CD1	PHE	A	44	108.627	61.162	50.555	1.00	23.33	A
ATOM	341	CD2	PHE	A	44	107.624	59.154	49.710	1.00	22.69	A
ATOM	342	CE1	PHE	A	44	107.424	61.514	51.193	1.00	22.52	A
ATOM	343	CE2	PHE	A	44	106.405	59.486	50.344	1.00	27.02	A
ATOM	344	CZ	PHE	A	44	106.306	60.674	51.083	1.00	27.40	A
ATOM	345	C	PHE	A	44	110.533	57.628	50.510	1.00	24.45	A
ATOM	346	O	PHE	A	44	110.059	57.605	51.647	1.00	18.55	A
ATOM	347	N	GLY	A	45	110.636	56.550	49.730	1.00	20.97	A
ATOM	348	CA	GLY	A	45	110.142	55.236	50.131	1.00	20.25	A
ATOM	349	C	GLY	A	45	109.064	54.826	49.136	1.00	23.29	A
ATOM	350	O	GLY	A	45	107.871	55.185	49.279	1.00	17.57	A
ATOM	351	N	LEU	A	46	109.465	54.095	48.104	1.00	20.22	A
ATOM	352	CA	LEU	A	46	108.525	53.666	47.089	1.00	18.57	A
ATOM	353	CB	LEU	A	46	109.243	52.881	45.977	1.00	27.58	A
ATOM	354	CG	LEU	A	46	108.444	52.315	44.770	1.00	35.06	A
ATOM	355	CD1	LEU	A	46	107.661	53.396	44.022	1.00	27.92	A
ATOM	356	CD2	LEU	A	46	109.443	51.614	43.809	1.00	32.82	A
ATOM	357	C	LEU	A	46	107.322	52.884	47.611	1.00	23.74	A
ATOM	358	O	LEU	A	46	106.255	52.927	46.995	1.00	19.46	A
ATOM	359	N	GLU	A	47	107.450	52.190	48.738	1.00	19.11	A
ATOM	360	CA	GLU	A	47	106.292	51.453	49.220	1.00	29.84	A
ATOM	361	CB	GLU	A	47	106.629	50.448	50.330	1.00	30.68	A
ATOM	362	CG	GLU	A	47	107.600	50.871	51.370	1.00	45.90	A
ATOM	363	CD	GLU	A	47	107.135	52.019	52.226	1.00	52.96	A
ATOM	364	OE1	GLU	A	47	105.927	52.017	52.597	1.00	60.59	A
ATOM	365	OE2	GLU	A	47	107.991	52.901	52.541	1.00	47.47	A
ATOM	366	C	GLU	A	47	105.151	52.350	49.678	1.00	27.56	A
ATOM	367	O	GLU	A	47	104.061	51.855	49.854	1.00	24.22	A
ATOM	368	N	LYS	A	48	105.403	53.655	49.861	1.00	26.01	A
ATOM	369	CA	LYS	A	48	104.340	54.594	50.262	1.00	20.77	A
ATOM	370	CB	LYS	A	48	104.924	55.863	50.888	1.00	20.15	A
ATOM	371	CG	LYS	A	48	105.694	55.636	52.167	1.00	19.21	A
ATOM	372	CD	LYS	A	48	106.344	56.939	52.656	1.00	20.50	A
ATOM	373	CE	LYS	A	48	107.190	56.673	53.891	1.00	30.14	A
ATOM	374	NZ	LYS	A	48	108.457	55.962	53.556	1.00	23.91	A
ATOM	375	C	LYS	A	48	103.513	55.013	49.059	1.00	19.66	A
ATOM	376	O	LYS	A	48	102.415	55.567	49.217	1.00	23.92	A
ATOM	377	N	ARG	A	49	104.005	54.750	47.850	1.00	17.52	A
ATOM	378	CA	ARG	A	49	103.257	55.178	46.655	1.00	21.83	A
ATOM	379	CB	ARG	A	49	104.048	54.879	45.360	1.00	16.40	A
ATOM	380	CG	ARG	A	49	103.443	55.612	44.111	1.00	14.73	A
ATOM	381	CD	ARG	A	49	104.410	55.661	42.916	1.00	21.52	A
ATOM	382	NE	ARG	A	49	103.924	56.478	41.815	1.00	16.66	A
ATOM	383	CZ	ARG	A	49	103.062	56.056	40.889	1.00	31.21	A

ATOM	384	NH1	ARG	A	49	102.592	54.803	40.922	1.00	20.87	A
ATOM	385	NH2	ARG	A	49	102.657	56.894	39.938	1.00	21.02	A
ATOM	386	C	ARG	A	49	101.826	54.612	46.536	1.00	24.68	A
ATOM	387	O	ARG	A	49	100.872	55.334	46.224	1.00	20.52	A
ATOM	388	N	GLN	A	50	101.681	53.313	46.785	1.00	31.61	A
ATOM	389	CA	GLN	A	50	100.398	52.629	46.691	1.00	24.84	A
ATOM	390	CB	GLN	A	50	100.531	51.187	47.168	1.00	33.17	A
ATOM	391	CG	GLN	A	50	100.197	50.169	46.142	1.00	46.59	A
ATOM	392	CD	GLN	A	50	98.794	50.305	45.608	1.00	42.68	A
ATOM	393	OE1	GLN	A	50	97.825	50.200	46.346	1.00	40.26	A
ATOM	394	NE2	GLN	A	50	98.684	50.542	44.308	1.00	47.02	A
ATOM	395	C	GLN	A	50	99.381	53.289	47.577	1.00	27.71	A
ATOM	396	O	GLN	A	50	98.257	53.562	47.157	1.00	18.05	A
ATOM	397	N	GLY	A	51	99.795	53.504	48.822	1.00	19.41	A
ATOM	398	CA	GLY	A	51	98.944	54.124	49.820	1.00	24.54	A
ATOM	399	C	GLY	A	51	98.517	55.489	49.329	1.00	27.23	A
ATOM	400	O	GLY	A	51	97.347	55.861	49.470	1.00	27.21	A
ATOM	401	N	ALA	A	52	99.444	56.233	48.723	1.00	21.82	A
ATOM	402	CA	ALA	A	52	99.089	57.561	48.220	1.00	21.64	A
ATOM	403	CB	ALA	A	52	100.343	58.319	47.777	1.00	20.17	A
ATOM	404	C	ALA	A	52	98.117	57.446	47.065	1.00	18.79	A
ATOM	405	O	ALA	A	52	97.209	58.265	46.947	1.00	21.57	A
ATOM	406	N	LEU	A	53	98.296	56.436	46.206	1.00	16.94	A
ATOM	407	CA	LEU	A	53	97.379	56.279	45.079	1.00	20.49	A
ATOM	408	CB	LEU	A	53	97.816	55.148	44.151	1.00	22.88	A
ATOM	409	CG	LEU	A	53	99.197	55.310	43.509	1.00	27.56	A
ATOM	410	CD1	LEU	A	53	99.526	54.081	42.643	1.00	28.51	A
ATOM	411	CD2	LEU	A	53	99.207	56.557	42.665	1.00	19.40	A
ATOM	412	C	LEU	A	53	95.966	56.027	45.571	1.00	22.20	A
ATOM	413	O	LEU	A	53	95.014	56.559	44.996	1.00	22.74	A
ATOM	414	N	GLU	A	54	95.838	55.241	46.643	1.00	20.38	A
ATOM	415	CA	GLU	A	54	94.542	54.937	47.247	1.00	22.21	A
ATOM	416	CB	GLU	A	54	94.705	53.920	48.404	1.00	32.94	A
ATOM	417	CG	GLU	A	54	95.023	52.489	47.951	1.00	41.26	A
ATOM	418	CD	GLU	A	54	95.587	51.579	49.071	1.00	48.52	A
ATOM	419	OE1	GLU	A	54	95.476	51.903	50.286	1.00	50.15	A
ATOM	420	OE2	GLU	A	54	96.141	50.514	48.717	1.00	50.30	A
ATOM	421	C	GLU	A	54	93.870	56.214	47.801	1.00	24.94	A
ATOM	422	O	GLU	A	54	92.644	56.351	47.710	1.00	21.97	A
ATOM	423	N	LEU	A	55	94.656	57.126	48.392	1.00	18.88	A
ATOM	424	CA	LEU	A	55	94.085	58.351	48.948	1.00	21.65	A
ATOM	425	CB	LEU	A	55	95.099	59.091	49.809	1.00	17.30	A
ATOM	426	CG	LEU	A	55	95.464	58.303	51.072	1.00	26.70	A
ATOM	427	CD1	LEU	A	55	96.576	59.072	51.841	1.00	25.33	A
ATOM	428	CD2	LEU	A	55	94.196	58.153	51.981	1.00	20.15	A
ATOM	429	C	LEU	A	55	93.646	59.229	47.802	1.00	18.82	A
ATOM	430	O	LEU	A	55	92.613	59.897	47.902	1.00	16.55	A
ATOM	431	N	ILE	A	56	94.413	59.218	46.712	1.00	15.91	A
ATOM	432	CA	ILE	A	56	94.065	60.024	45.513	1.00	16.74	A
ATOM	433	CB	ILE	A	56	95.151	59.930	44.390	1.00	21.15	A
ATOM	434	CG2	ILE	A	56	94.710	60.691	43.120	1.00	25.29	A
ATOM	435	CG1	ILE	A	56	96.461	60.644	44.806	1.00	20.28	A
ATOM	436	CD1	ILE	A	56	96.234	61.948	45.382	1.00	40.37	A
ATOM	437	C	ILE	A	56	92.723	59.508	44.945	1.00	25.52	A
ATOM	438	O	ILE	A	56	91.816	60.297	44.615	1.00	18.85	A

ATOM	439	N	LYS	A	57	92.589	58.183	44.822	1.00	20.21	A
ATOM	440	CA	LYS	A	57	91.354	57.595	44.308	1.00	19.21	A
ATOM	441	CB	LYS	A	57	91.496	56.088	44.221	1.00	26.24	A
ATOM	442	CG	LYS	A	57	90.244	55.363	43.763	1.00	37.40	A
ATOM	443	CD	LYS	A	57	90.531	53.831	43.577	1.00	39.50	A
ATOM	444	CE	LYS	A	57	89.290	53.088	43.091	1.00	45.08	A
ATOM	445	NZ	LYS	A	57	89.516	51.637	42.936	1.00	50.42	A
ATOM	446	C	LYS	A	57	90.192	57.952	45.242	1.00	23.30	A
ATOM	447	O	LYS	A	57	89.082	58.273	44.789	1.00	20.92	A
ATOM	448	N	LYS	A	58	90.445	57.902	46.550	1.00	16.98	A
ATOM	449	CA	LYS	A	58	89.421	58.260	47.513	1.00	17.12	A
ATOM	450	CB	LYS	A	58	89.971	58.041	48.937	1.00	18.85	A
ATOM	451	CG	LYS	A	58	88.973	58.307	50.047	1.00	25.94	A
ATOM	452	CD	LYS	A	58	89.491	57.947	51.437	1.00	35.63	A
ATOM	453	CE	LYS	A	58	88.639	58.677	52.501	1.00	42.54	A
ATOM	454	NZ	LYS	A	58	88.728	58.038	53.858	1.00	50.94	A
ATOM	455	C	LYS	A	58	89.011	59.749	47.300	1.00	25.76	A
ATOM	456	O	LYS	A	58	87.808	60.095	47.288	1.00	22.91	A
ATOM	457	N	GLY	A	59	89.999	60.629	47.099	1.00	21.23	A
ATOM	458	CA	GLY	A	59	89.691	62.041	46.894	1.00	23.41	A
ATOM	459	C	GLY	A	59	88.819	62.247	45.664	1.00	25.51	A
ATOM	460	O	GLY	A	59	87.820	62.978	45.683	1.00	21.04	A
ATOM	461	N	TYR	A	60	89.213	61.576	44.588	1.00	21.05	A
ATOM	462	CA	TYR	A	60	88.517	61.642	43.312	1.00	23.66	A
ATOM	463	CB	TYR	A	60	89.244	60.776	42.296	1.00	13.71	A
ATOM	464	CG	TYR	A	60	88.456	60.499	41.039	1.00	25.98	A
ATOM	465	CD1	TYR	A	60	88.276	61.495	40.082	1.00	22.56	A
ATOM	466	CE1	TYR	A	60	87.570	61.250	38.915	1.00	26.16	A
ATOM	467	CD2	TYR	A	60	87.893	59.223	40.792	1.00	27.02	A
ATOM	468	CE2	TYR	A	60	87.180	58.966	39.610	1.00	23.07	A
ATOM	469	CZ	TYR	A	60	87.027	59.994	38.677	1.00	27.86	A
ATOM	470	OH	TYR	A	60	86.347	59.798	37.490	1.00	19.73	A
ATOM	471	C	TYR	A	60	87.089	61.131	43.448	1.00	23.97	A
ATOM	472	O	TYR	A	60	86.129	61.776	43.024	1.00	16.61	A
ATOM	473	N	THR	A	61	86.947	59.954	44.029	1.00	22.77	A
ATOM	474	CA	THR	A	61	85.615	59.365	44.185	1.00	22.30	A
ATOM	475	CB	THR	A	61	85.739	58.003	44.849	1.00	30.49	A
ATOM	476	OG1	THR	A	61	86.448	57.145	43.960	1.00	31.94	A
ATOM	477	CG2	THR	A	61	84.371	57.401	45.164	1.00	42.36	A
ATOM	478	C	THR	A	61	84.724	60.246	45.008	1.00	23.97	A
ATOM	479	O	THR	A	61	83.554	60.480	44.668	1.00	22.40	A
ATOM	480	N	GLN	A	62	85.267	60.743	46.108	1.00	20.42	A
ATOM	481	CA	GLN	A	62	84.476	61.619	46.958	1.00	23.93	A
ATOM	482	CB	GLN	A	62	85.255	61.966	48.242	1.00	24.47	A
ATOM	483	CG	GLN	A	62	85.293	60.776	49.207	1.00	26.29	A
ATOM	484	CD	GLN	A	62	86.265	60.940	50.385	1.00	27.78	A
ATOM	485	OE1	GLN	A	62	86.263	60.126	51.289	1.00	27.57	A
ATOM	486	NE2	GLN	A	62	87.098	61.980	50.362	1.00	32.36	A
ATOM	487	C	GLN	A	62	84.037	62.885	46.215	1.00	19.82	A
ATOM	488	O	GLN	A	62	82.903	63.334	46.374	1.00	21.86	A
ATOM	489	N	GLN	A	63	84.910	63.441	45.382	1.00	20.60	A
ATOM	490	CA	GLN	A	63	84.569	64.669	44.667	1.00	23.75	A
ATOM	491	CB	GLN	A	63	85.772	65.168	43.862	1.00	17.42	A
ATOM	492	CG	GLN	A	63	85.669	66.602	43.360	1.00	15.84	A
ATOM	493	CD	GLN	A	63	85.470	67.642	44.449	1.00	18.31	A

ATOM	494	OE1	GLN	A	63	85.851	67.455	45.610	1.00	15.34	A
ATOM	495	NE2	GLN	A	63	84.900	68.779	44.062	1.00	17.92	A
ATOM	496	C	GLN	A	63	83.371	64.460	43.721	1.00	27.22	A
ATOM	497	O	GLN	A	63	82.590	65.388	43.471	1.00	16.84	A
ATOM	498	N	LEU	A	64	83.223	63.249	43.201	1.00	18.15	A
ATOM	499	CA	LEU	A	64	82.113	62.984	42.289	1.00	20.34	A
ATOM	500	CB	LEU	A	64	82.194	61.562	41.738	1.00	20.67	A
ATOM	501	CG	LEU	A	64	83.460	61.266	40.904	1.00	29.97	A
ATOM	502	CD1	LEU	A	64	83.341	59.848	40.328	1.00	28.53	A
ATOM	503	CD2	LEU	A	64	83.645	62.308	39.769	1.00	25.04	A
ATOM	504	C	LEU	A	64	80.781	63.214	42.971	1.00	20.30	A
ATOM	505	O	LEU	A	64	79.818	63.568	42.314	1.00	23.21	A
ATOM	506	N	ALA	A	65	80.708	63.015	44.288	1.00	15.07	A
ATOM	507	CA	ALA	A	65	79.459	63.267	44.975	1.00	19.06	A
ATOM	508	CB	ALA	A	65	79.595	62.955	46.447	1.00	19.25	A
ATOM	509	C	ALA	A	65	79.010	64.717	44.790	1.00	19.22	A
ATOM	510	O	ALA	A	65	77.864	65.042	45.087	1.00	24.93	A
ATOM	511	N	PHE	A	66	79.895	65.592	44.314	1.00	22.94	A
ATOM	512	CA	PHE	A	66	79.533	67.015	44.134	1.00	22.02	A
ATOM	513	CB	PHE	A	66	80.481	67.908	44.943	1.00	21.43	A
ATOM	514	CG	PHE	A	66	80.548	67.511	46.386	1.00	24.76	A
ATOM	515	CD1	PHE	A	66	79.542	67.914	47.287	1.00	21.43	A
ATOM	516	CD2	PHE	A	66	81.573	66.657	46.840	1.00	20.02	A
ATOM	517	CE1	PHE	A	66	79.555	67.467	48.605	1.00	22.96	A
ATOM	518	CE2	PHE	A	66	81.594	66.203	48.162	1.00	18.70	A
ATOM	519	CZ	PHE	A	66	80.584	66.611	49.049	1.00	21.49	A
ATOM	520	C	PHE	A	66	79.511	67.461	42.693	1.00	17.64	A
ATOM	521	O	PHE	A	66	79.405	68.673	42.389	1.00	18.14	A
ATOM	522	N	ARG	A	67	79.606	66.481	41.796	1.00	21.16	A
ATOM	523	CA	ARG	A	67	79.541	66.745	40.354	1.00	23.23	A
ATOM	524	CB	ARG	A	67	79.971	65.496	39.598	1.00	18.11	A
ATOM	525	CG	ARG	A	67	79.896	65.665	38.107	1.00	28.17	A
ATOM	526	CD	ARG	A	67	80.315	64.386	37.363	1.00	25.25	A
ATOM	527	NE	ARG	A	67	80.344	64.619	35.923	1.00	25.71	A
ATOM	528	CZ	ARG	A	67	80.004	63.715	35.012	1.00	26.53	A
ATOM	529	NH1	ARG	A	67	79.601	62.496	35.388	1.00	23.05	A
ATOM	530	NH2	ARG	A	67	80.089	64.028	33.724	1.00	16.97	A
ATOM	531	C	ARG	A	67	78.055	67.034	40.044	1.00	25.46	A
ATOM	532	O	ARG	A	67	77.223	66.244	40.427	1.00	18.92	A
ATOM	533	N	GLN	A	68	77.716	68.150	39.395	1.00	21.57	A
ATOM	534	CA	GLN	A	68	76.305	68.440	39.084	1.00	20.68	A
ATOM	535	CB	GLN	A	68	76.073	69.964	39.186	1.00	23.31	A
ATOM	536	CG	GLN	A	68	76.532	70.448	40.570	1.00	17.98	A
ATOM	537	CD	GLN	A	68	75.990	71.790	40.937	1.00	25.72	A
ATOM	538	OE1	GLN	A	68	75.464	72.528	40.084	1.00	23.05	A
ATOM	539	NE2	GLN	A	68	76.132	72.140	42.206	1.00	15.43	A
ATOM	540	C	GLN	A	68	75.871	67.887	37.722	1.00	16.68	A
ATOM	541	O	GLN	A	68	76.704	67.367	36.998	1.00	19.76	A
ATOM	542	N	PRO	A	69	74.563	67.945	37.368	1.00	22.91	A
ATOM	543	CD	PRO	A	69	73.385	68.286	38.198	1.00	21.74	A
ATOM	544	CA	PRO	A	69	74.144	67.408	36.046	1.00	20.68	A
ATOM	545	CB	PRO	A	69	72.628	67.698	35.995	1.00	17.83	A
ATOM	546	CG	PRO	A	69	72.208	67.532	37.454	1.00	16.18	A
ATOM	547	C	PRO	A	69	74.886	68.078	34.892	1.00	23.73	A
ATOM	548	O	PRO	A	69	75.152	67.467	33.875	1.00	23.28	A

ATOM	549	N	SER	A	70	75.246	69.340	35.086	1.00	24.11	A
ATOM	550	CA	SER	A	70	75.975	70.114	34.092	1.00	23.11	A
ATOM	551	CB	SER	A	70	76.000	71.580	34.528	1.00	20.68	A
ATOM	552	OG	SER	A	70	76.662	71.709	35.793	1.00	27.57	A
ATOM	553	C	SER	A	70	77.436	69.654	33.942	1.00	27.84	A
ATOM	554	O	SER	A	70	78.127	70.080	33.021	1.00	24.67	A
ATOM	555	N	SER	A	71	77.885	68.805	34.868	1.00	19.80	A
ATOM	556	CA	SER	A	71	79.288	68.333	34.971	1.00	20.11	A
ATOM	557	CB	SER	A	71	79.953	68.052	33.613	1.00	22.15	A
ATOM	558	OG	SER	A	71	79.498	66.853	33.011	1.00	21.54	A
ATOM	559	C	SER	A	71	80.131	69.401	35.702	1.00	20.52	A
ATOM	560	O	SER	A	71	81.329	69.262	35.782	1.00	19.50	A
ATOM	561	N	ALA	A	72	79.522	70.477	36.199	1.00	19.13	A
ATOM	562	CA	ALA	A	72	80.273	71.479	36.973	1.00	21.30	A
ATOM	563	CB	ALA	A	72	79.665	72.897	36.823	1.00	16.76	A
ATOM	564	C	ALA	A	72	80.250	71.064	38.447	1.00	24.51	A
ATOM	565	O	ALA	A	72	79.540	70.122	38.840	1.00	20.95	A
ATOM	566	N	PHE	A	73	81.026	71.773	39.266	1.00	22.89	A
ATOM	567	CA	PHE	A	73	81.113	71.484	40.695	1.00	19.84	A
ATOM	568	CB	PHE	A	73	82.541	70.958	41.056	1.00	16.24	A
ATOM	569	CG	PHE	A	73	82.890	69.625	40.409	1.00	17.75	A
ATOM	570	CD1	PHE	A	73	83.265	69.554	39.067	1.00	14.21	A
ATOM	571	CD2	PHE	A	73	82.791	68.439	41.140	1.00	21.80	A
ATOM	572	CE1	PHE	A	73	83.527	68.310	38.447	1.00	18.43	A
ATOM	573	CE2	PHE	A	73	83.048	67.196	40.546	1.00	20.67	A
ATOM	574	CZ	PHE	A	73	83.418	67.115	39.190	1.00	17.64	A
ATOM	575	C	PHE	A	73	80.846	72.708	41.561	1.00	15.55	A
ATOM	576	O	PHE	A	73	81.079	73.846	41.134	1.00	17.42	A
ATOM	577	N	ALA	A	74	80.392	72.437	42.787	1.00	18.86	A
ATOM	578	CA	ALA	A	74	80.196	73.440	43.842	1.00	21.20	A
ATOM	579	CB	ALA	A	74	78.774	74.076	43.782	1.00	14.22	A
ATOM	580	C	ALA	A	74	80.381	72.705	45.171	1.00	19.11	A
ATOM	581	O	ALA	A	74	80.364	71.471	45.211	1.00	23.95	A
ATOM	582	N	ALA	A	75	80.579	73.456	46.259	1.00	17.13	A
ATOM	583	CA	ALA	A	75	80.738	72.883	47.584	1.00	21.11	A
ATOM	584	CB	ALA	A	75	80.813	73.959	48.592	1.00	12.54	A
ATOM	585	C	ALA	A	75	79.600	71.944	47.961	1.00	19.04	A
ATOM	586	O	ALA	A	75	79.821	70.901	48.589	1.00	18.22	A
ATOM	587	N	PHE	A	76	78.386	72.317	47.591	1.00	20.53	A
ATOM	588	CA	PHE	A	76	77.202	71.519	47.920	1.00	15.82	A
ATOM	589	CB	PHE	A	76	76.420	72.195	49.053	1.00	17.12	A
ATOM	590	CG	PHE	A	76	77.249	72.514	50.258	1.00	26.60	A
ATOM	591	CD1	PHE	A	76	77.723	71.505	51.098	1.00	27.70	A
ATOM	592	CD2	PHE	A	76	77.576	73.824	50.551	1.00	22.87	A
ATOM	593	CE1	PHE	A	76	78.512	71.807	52.212	1.00	22.16	A
ATOM	594	CE2	PHE	A	76	78.367	74.125	51.667	1.00	28.08	A
ATOM	595	CZ	PHE	A	76	78.832	73.128	52.490	1.00	23.72	A
ATOM	596	C	PHE	A	76	76.343	71.444	46.674	1.00	23.48	A
ATOM	597	O	PHE	A	76	76.308	72.404	45.866	1.00	15.81	A
ATOM	598	N	VAL	A	77	75.639	70.327	46.465	1.00	19.15	A
ATOM	599	CA	VAL	A	77	74.845	70.141	45.255	1.00	23.84	A
ATOM	600	CB	VAL	A	77	74.279	68.688	45.144	1.00	24.38	A
ATOM	601	CG1	VAL	A	77	75.456	67.682	44.930	1.00	20.82	A
ATOM	602	CG2	VAL	A	77	73.465	68.349	46.390	1.00	19.64	A
ATOM	603	C	VAL	A	77	73.701	71.122	45.082	1.00	20.75	A

ATOM	654	O	VAL	A	77	73.201	71.320	43.973	1.00	24.71	A
ATOM	655	N	LYS	A	78	73.302	71.723	46.184	1.00	15.92	A
ATOM	656	CA	LYS	A	78	72.245	72.712	46.200	1.00	28.31	A
ATOM	657	CB	LYS	A	78	71.642	72.818	47.590	1.00	31.59	A
ATOM	658	CG	LYS	A	78	70.888	72.559	47.898	1.00	52.94	A
ATOM	659	CD	LYS	A	78	69.877	71.719	48.992	1.00	60.83	A
ATOM	660	CE	LYS	A	78	68.914	70.543	48.967	1.00	61.05	A
ATOM	661	NZ	LYS	A	78	68.246	70.353	47.672	1.00	30.69	A
ATOM	662	C	LYS	A	78	72.755	74.071	45.823	1.00	26.47	A
ATOM	663	O	LYS	A	78	71.956	74.971	45.569	1.00	24.70	A
ATOM	664	N	ARG	A	79	74.080	74.223	45.818	1.00	20.39	A
ATOM	665	CA	ARG	A	79	74.723	75.499	45.514	1.00	21.78	A
ATOM	666	CB	ARG	A	79	76.013	75.592	46.349	1.00	19.49	A
ATOM	667	CG	ARG	A	79	76.859	76.847	46.120	1.00	23.95	A
ATOM	668	CD	ARG	A	79	78.098	76.897	47.058	1.00	20.40	A
ATOM	669	NE	ARG	A	79	78.758	78.204	47.005	1.00	25.41	A
ATOM	670	CZ	ARG	A	79	78.559	79.167	47.899	1.00	30.60	A
ATOM	671	NH1	ARG	A	79	77.724	78.956	48.915	1.00	29.61	A
ATOM	672	NH2	ARG	A	79	79.177	80.338	47.780	1.00	23.38	A
ATOM	673	C	ARG	A	79	75.036	75.716	44.030	1.00	21.79	A
ATOM	674	O	ARG	A	79	75.417	74.764	43.332	1.00	19.63	A
ATOM	675	N	ALA	A	80	74.877	76.967	43.553	1.00	21.57	A
ATOM	676	CA	ALA	A	80	75.180	77.331	42.159	1.00	26.40	A
ATOM	677	CB	ALA	A	80	74.960	78.868	41.923	1.00	22.62	A
ATOM	678	C	ALA	A	80	76.659	76.953	41.914	1.00	20.22	A
ATOM	679	O	ALA	A	80	77.519	77.179	42.780	1.00	23.83	A
ATOM	680	N	PRO	A	81	76.959	76.365	40.744	1.00	23.02	A
ATOM	681	CD	PRO	A	81	75.984	76.235	39.641	1.00	22.02	A
ATOM	682	CA	PRO	A	81	78.301	75.909	40.337	1.00	20.18	A
ATOM	683	CB	PRO	A	81	78.046	75.207	38.995	1.00	23.34	A
ATOM	684	CG	PRO	A	81	76.879	75.999	38.416	1.00	25.62	A
ATOM	685	C	PRO	A	81	79.370	76.990	40.238	1.00	24.53	A
ATOM	686	O	PRO	A	81	79.132	78.085	39.736	1.00	18.24	A
ATOM	687	N	SER	A	82	80.560	76.677	40.736	1.00	18.76	A
ATOM	688	CA	SER	A	82	81.648	77.630	40.669	1.00	15.88	A
ATOM	689	CB	SER	A	82	82.494	77.549	41.942	1.00	19.09	A
ATOM	690	OG	SER	A	82	83.781	78.102	41.725	1.00	15.72	A
ATOM	691	C	SER	A	82	82.529	77.411	39.437	1.00	18.93	A
ATOM	692	O	SER	A	82	82.981	76.286	39.114	1.00	17.23	A
ATOM	693	N	THR	A	83	82.762	78.494	38.725	1.00	17.20	A
ATOM	694	CA	THR	A	83	83.628	78.442	37.544	1.00	16.78	A
ATOM	695	CB	THR	A	83	83.692	79.829	36.868	1.00	19.03	A
ATOM	696	OG1	THR	A	83	82.397	80.168	36.390	1.00	20.73	A
ATOM	697	CG2	THR	A	83	84.666	79.840	35.692	1.00	17.21	A
ATOM	698	C	THR	A	83	85.060	78.069	38.027	1.00	20.11	A
ATOM	699	O	THR	A	83	85.740	77.214	37.446	1.00	15.09	A
ATOM	700	N	TRP	A	84	85.514	78.745	39.084	1.00	16.86	A
ATOM	701	CA	TRP	A	84	86.839	78.483	39.627	1.00	24.71	A
ATOM	702	CB	TRP	A	84	87.171	79.427	40.780	1.00	16.82	A
ATOM	703	CG	TRP	A	84	88.624	79.255	41.247	1.00	17.86	A
ATOM	704	CD2	TRP	A	84	89.106	78.315	42.218	1.00	16.17	A
ATOM	705	CE2	TRP	A	84	90.510	78.464	42.284	1.00	22.04	A
ATOM	706	CE3	TRP	A	84	88.486	77.366	43.035	1.00	17.61	A
ATOM	707	CD1	TRP	A	84	89.727	79.915	40.783	1.00	23.03	A
ATOM	708	NE1	TRP	A	84	90.859	79.447	41.405	1.00	16.07	A

ATOM	659	CZ2	TRP	A	84	91.308	77.686	43.141	1.00	21.59	A
ATOM	660	CZ3	TRP	A	84	89.279	76.595	43.892	1.00	21.38	A
ATOM	661	CH2	TRP	A	84	90.670	76.759	43.936	1.00	17.83	A
ATOM	662	C	TRP	A	84	87.001	77.049	40.136	1.00	22.89	A
ATOM	663	O	TRP	A	84	87.973	76.398	39.800	1.00	18.84	A
ATOM	664	N	LEU	A	85	86.065	76.561	40.949	1.00	23.94	A
ATOM	665	CA	LEU	A	85	86.175	75.193	41.495	1.00	19.54	A
ATOM	666	CB	LEU	A	85	85.011	74.891	42.475	1.00	14.42	A
ATOM	667	CG	LEU	A	85	85.115	73.580	43.258	1.00	19.45	A
ATOM	668	CD1	LEU	A	85	86.371	73.566	44.197	1.00	11.14	A
ATOM	669	CD2	LEU	A	85	83.825	73.422	44.060	1.00	18.37	A
ATOM	670	C	LEU	A	85	86.175	74.195	40.356	1.00	24.50	A
ATOM	671	O	LEU	A	85	86.994	73.257	40.330	1.00	19.38	A
ATOM	672	N	THR	A	86	85.285	74.413	39.383	1.00	16.67	A
ATOM	673	CA	THR	A	86	85.226	73.494	38.279	1.00	18.11	A
ATOM	674	CB	THR	A	86	84.068	73.818	37.357	1.00	17.96	A
ATOM	675	OG1	THR	A	86	82.871	73.696	38.127	1.00	12.56	A
ATOM	676	CG2	THR	A	86	84.007	72.851	36.202	1.00	14.63	A
ATOM	677	C	THR	A	86	86.534	73.480	37.569	1.00	18.80	A
ATOM	678	O	THR	A	86	87.057	72.395	37.283	1.00	15.97	A
ATOM	679	N	ALA	A	87	87.111	74.657	37.315	1.00	15.61	A
ATOM	680	CA	ALA	A	87	88.422	74.679	36.645	1.00	21.28	A
ATOM	681	CB	ALA	A	87	88.812	76.132	36.265	1.00	17.13	A
ATOM	682	C	ALA	A	87	89.532	74.068	37.535	1.00	21.82	A
ATOM	683	O	ALA	A	87	90.531	73.527	37.036	1.00	18.47	A
ATOM	684	N	TYR	A	88	89.400	74.203	38.845	1.00	16.96	A
ATOM	685	CA	TYR	A	88	90.439	73.637	39.708	1.00	19.62	A
ATOM	686	CB	TYR	A	88	90.324	74.155	41.140	1.00	17.51	A
ATOM	687	CG	TYR	A	88	91.533	73.749	41.989	1.00	17.09	A
ATOM	688	CD1	TYR	A	88	92.843	73.975	41.528	1.00	17.38	A
ATOM	689	CE1	TYR	A	88	93.947	73.554	42.259	1.00	18.76	A
ATOM	690	CD2	TYR	A	88	91.366	73.093	43.214	1.00	20.06	A
ATOM	691	CE2	TYR	A	88	92.475	72.663	43.971	1.00	20.12	A
ATOM	692	CZ	TYR	A	88	93.746	72.903	43.488	1.00	20.21	A
ATOM	693	OH	TYR	A	88	94.817	72.537	44.255	1.00	13.27	A
ATOM	694	C	TYR	A	88	90.318	72.119	39.706	1.00	21.43	A
ATOM	695	O	TYR	A	88	91.316	71.390	39.776	1.00	16.93	A
ATOM	696	N	VAL	A	89	89.092	71.625	39.636	1.00	19.57	A
ATOM	697	CA	VAL	A	89	88.949	70.192	39.599	1.00	19.82	A
ATOM	698	CB	VAL	A	89	87.486	69.796	39.599	1.00	18.50	A
ATOM	699	CG1	VAL	A	89	87.331	68.263	39.251	1.00	15.01	A
ATOM	700	CG2	VAL	A	89	86.918	70.101	40.995	1.00	13.83	A
ATOM	701	C	VAL	A	89	89.659	69.678	38.349	1.00	23.95	A
ATOM	702	O	VAL	A	89	90.348	68.656	38.395	1.00	18.30	A
ATOM	703	N	VAL	A	90	89.491	70.382	37.232	1.00	17.40	A
ATOM	704	CA	VAL	A	90	90.160	69.981	35.990	1.00	18.85	A
ATOM	705	CB	VAL	A	90	89.724	70.929	34.791	1.00	19.41	A
ATOM	706	CG1	VAL	A	90	90.600	70.715	33.553	1.00	13.53	A
ATOM	707	CG2	VAL	A	90	88.248	70.648	34.399	1.00	17.29	A
ATOM	708	C	VAL	A	90	91.703	70.043	36.175	1.00	19.91	A
ATOM	709	O	VAL	A	90	92.452	69.188	35.696	1.00	20.47	A
ATOM	710	N	LYS	A	91	92.181	71.075	36.858	1.00	20.83	A
ATOM	711	CA	LYS	A	91	93.614	71.240	37.046	1.00	23.83	A
ATOM	712	CB	LYS	A	91	93.861	72.579	37.741	1.00	21.45	A
ATOM	713	CG	LYS	A	91	95.232	73.277	37.527	1.00	24.31	A

ATOM	714	CD	LYS	A	91	95.603	73.978	38.817	1.00	28.86	A
ATOM	715	CE	LYS	A	91	96.264	75.359	38.681	1.00	41.38	A
ATOM	716	NZ	LYS	A	91	97.276	75.477	37.603	1.00	23.09	A
ATOM	717	C	LYS	A	91	94.176	70.090	37.904	1.00	22.83	A
ATOM	718	O	LYS	A	91	95.288	69.615	37.659	1.00	28.75	A
ATOM	719	N	VAL	A	92	93.422	69.641	38.908	1.00	16.52	A
ATOM	720	CA	VAL	A	92	93.938	68.571	39.767	1.00	15.54	A
ATOM	721	CB	VAL	A	92	93.220	68.564	41.134	1.00	14.74	A
ATOM	722	CG1	VAL	A	92	93.669	67.333	41.957	1.00	12.97	A
ATOM	723	CG2	VAL	A	92	93.531	69.882	41.912	1.00	15.57	A
ATOM	724	C	VAL	A	92	93.780	67.195	39.100	1.00	22.13	A
ATOM	725	O	VAL	A	92	94.735	66.398	39.027	1.00	19.97	A
ATOM	726	N	PHE	A	93	92.575	66.936	38.599	1.00	15.35	A
ATOM	727	CA	PHE	A	93	92.262	65.649	37.986	1.00	21.59	A
ATOM	728	CB	PHE	A	93	90.780	65.619	37.538	1.00	20.43	A
ATOM	729	CG	PHE	A	93	89.762	65.399	38.658	1.00	21.63	A
ATOM	730	CD1	PHE	A	93	90.101	65.531	40.003	1.00	22.34	A
ATOM	731	CD2	PHE	A	93	88.435	65.083	38.327	1.00	25.57	A
ATOM	732	CE1	PHE	A	93	89.146	65.347	41.015	1.00	18.59	A
ATOM	733	CE2	PHE	A	93	87.474	64.900	39.309	1.00	16.00	A
ATOM	734	CZ	PHE	A	93	87.827	65.034	40.660	1.00	18.70	A
ATOM	735	C	PHE	A	93	93.183	65.348	36.778	1.00	20.69	A
ATOM	736	O	PHE	A	93	93.572	64.201	36.582	1.00	22.65	A
ATOM	737	N	SER	A	94	93.516	66.364	35.975	1.00	19.95	A
ATOM	738	CA	SER	A	94	94.382	66.192	34.795	1.00	23.79	A
ATOM	739	CB	SER	A	94	94.563	67.526	34.040	1.00	23.74	A
ATOM	740	OG	SER	A	94	93.351	67.930	33.393	1.00	23.03	A
ATOM	741	C	SER	A	94	95.759	65.623	35.169	1.00	29.47	A
ATOM	742	O	SER	A	94	96.379	64.867	34.406	1.00	24.55	A
ATOM	743	N	LEU	A	95	96.230	65.998	36.346	1.00	25.17	A
ATOM	744	CA	LEU	A	95	97.500	65.515	36.858	1.00	29.40	A
ATOM	745	CB	LEU	A	95	97.953	66.430	37.992	1.00	32.98	A
ATOM	746	CG	LEU	A	95	99.047	67.438	37.643	1.00	41.49	A
ATOM	747	CD1	LEU	A	95	98.732	68.151	36.358	1.00	36.09	A
ATOM	748	CD2	LEU	A	95	99.244	68.378	38.800	1.00	40.51	A
ATOM	749	C	LEU	A	95	97.413	64.064	37.368	1.00	31.25	A
ATOM	750	O	LEU	A	95	98.433	63.376	37.493	1.00	24.33	A
ATOM	751	N	ALA	A	96	96.203	63.614	37.685	1.00	28.03	A
ATOM	752	CA	ALA	A	96	95.991	62.260	38.208	1.00	27.75	A
ATOM	753	CB	ALA	A	96	94.901	62.301	39.286	1.00	26.88	A
ATOM	754	C	ALA	A	96	95.629	61.204	37.157	1.00	29.48	A
ATOM	755	O	ALA	A	96	95.529	60.013	37.479	1.00	25.41	A
ATOM	756	N	VAL	A	97	95.447	61.639	35.910	1.00	25.39	A
ATOM	757	CA	VAL	A	97	95.035	60.759	34.802	1.00	29.11	A
ATOM	758	CB	VAL	A	97	95.034	61.571	33.480	1.00	28.78	A
ATOM	759	CG1	VAL	A	97	95.057	60.663	32.321	1.00	38.20	A
ATOM	760	CG2	VAL	A	97	93.748	62.496	33.422	1.00	34.13	A
ATOM	761	C	VAL	A	97	96.813	59.424	34.636	1.00	33.92	A
ATOM	762	O	VAL	A	97	95.222	58.281	34.289	1.00	31.47	A
ATOM	763	N	ASN	A	98	97.124	59.457	34.848	1.00	21.59	A
ATOM	764	CA	ASN	A	98	97.923	58.240	34.770	1.00	36.51	A
ATOM	765	CB	ASN	A	98	99.222	58.471	33.983	1.00	36.15	A
ATOM	766	CG	ASN	A	98	98.971	58.837	32.510	1.00	36.17	A
ATOM	767	OD1	ASN	A	98	98.119	58.252	31.844	1.00	38.38	A
ATOM	768	ND2	ASN	A	98	99.730	59.805	32.007	1.00	40.71	A

ATOM	769	C	ASN	A	98	98.260	57.700	36.178	1.00	37.38	A
ATOM	770	O	ASN	A	98	99.138	56.844	36.316	1.00	31.38	A
ATOM	771	N	LEU	A	99	97.562	58.205	37.205	1.00	25.80	A
ATOM	772	CA	LEU	A	99	97.763	57.760	38.592	1.00	34.00	A
ATOM	773	CB	LEU	A	99	97.747	58.936	39.580	1.00	23.10	A
ATOM	774	CG	LEU	A	99	98.867	59.966	39.407	1.00	26.85	A
ATOM	775	CD1	LEU	A	99	98.812	61.017	40.508	1.00	25.56	A
ATOM	776	CD2	LEU	A	99	100.191	59.231	39.390	1.00	29.12	A
ATOM	777	C	LEU	A	99	96.656	56.804	38.994	1.00	34.25	A
ATOM	778	O	LEU	A	99	96.911	55.782	39.629	1.00	29.94	A
ATOM	779	N	ILE	A	100	95.431	57.169	38.623	1.00	24.08	A
ATOM	780	CA	ILE	A	100	94.232	56.407	38.913	1.00	28.23	A
ATOM	781	CB	ILE	A	100	93.446	57.007	40.119	1.00	26.92	A
ATOM	782	CG2	ILE	A	100	94.300	56.986	41.388	1.00	21.39	A
ATOM	783	CG1	ILE	A	100	93.022	58.457	39.786	1.00	22.04	A
ATOM	784	CD1	ILE	A	100	91.965	59.043	40.791	1.00	21.31	A
ATOM	785	C	ILE	A	100	93.340	56.511	37.684	1.00	28.89	A
ATOM	786	O	ILE	A	100	93.676	57.218	36.738	1.00	25.36	A
ATOM	787	N	ALA	A	101	92.195	55.834	37.701	1.00	21.87	A
ATOM	788	CA	ALA	A	101	91.278	55.891	36.563	1.00	25.41	A
ATOM	789	CB	ALA	A	101	90.323	54.656	36.557	1.00	29.20	A
ATOM	790	C	ALA	A	101	90.426	57.148	36.639	1.00	27.34	A
ATOM	791	O	ALA	A	101	89.546	57.235	37.493	1.00	27.43	A
ATOM	792	N	ILE	A	102	90.676	58.121	35.774	1.00	25.35	A
ATOM	793	CA	ILE	A	102	89.837	59.308	35.794	1.00	26.53	A
ATOM	794	CB	ILE	A	102	90.666	60.596	35.788	1.00	30.43	A
ATOM	795	CG2	ILE	A	102	89.775	61.805	35.343	1.00	26.72	A
ATOM	796	CG1	ILE	A	102	91.165	60.849	37.221	1.00	33.11	A
ATOM	797	CD1	ILE	A	102	92.470	61.458	37.221	1.00	45.56	A
ATOM	798	C	ILE	A	102	88.919	59.248	34.585	1.00	22.33	A
ATOM	799	O	ILE	A	102	89.378	59.106	33.461	1.00	26.71	A
ATOM	800	N	ASP	A	103	87.621	59.318	34.836	1.00	26.27	A
ATOM	801	CA	ASP	A	103	86.616	59.227	33.776	1.00	25.84	A
ATOM	802	CB	ASP	A	103	85.231	59.056	34.425	1.00	25.81	A
ATOM	803	CG	ASP	A	103	84.114	58.863	33.403	1.00	34.26	A
ATOM	804	OD1	ASP	A	103	84.361	59.023	32.187	1.00	25.53	A
ATOM	805	OD2	ASP	A	103	82.979	58.551	33.828	1.00	39.65	A
ATOM	806	C	ASP	A	103	86.642	60.484	32.900	1.00	24.26	A
ATOM	807	O	ASP	A	103	86.385	61.577	33.381	1.00	26.29	A
ATOM	808	N	SER	A	104	86.972	60.331	31.627	1.00	24.09	A
ATOM	809	CA	SER	A	104	87.010	61.465	30.700	1.00	30.37	A
ATOM	810	CB	SER	A	104	87.490	60.999	29.333	1.00	35.62	A
ATOM	811	OG	SER	A	104	88.890	60.808	29.371	1.00	42.20	A
ATOM	812	C	SER	A	104	85.689	62.219	30.544	1.00	27.77	A
ATOM	813	O	SER	A	104	85.679	63.399	30.237	1.00	26.73	A
ATOM	814	N	GLN	A	105	84.576	61.534	30.741	1.00	26.58	A
ATOM	815	CA	GLN	A	105	83.264	62.158	30.673	1.00	31.05	A
ATOM	816	CB	GLN	A	105	82.162	61.141	30.991	1.00	33.79	A
ATOM	817	CG	GLN	A	105	81.964	60.052	29.984	1.00	45.91	A
ATOM	818	CD	GLN	A	105	81.570	60.627	28.655	1.00	53.89	A
ATOM	819	OE1	GLN	A	105	82.400	61.212	27.938	1.00	55.25	A
ATOM	820	NE2	GLN	A	105	80.286	60.499	28.320	1.00	55.15	A
ATOM	821	C	GLN	A	105	83.227	63.209	31.778	1.00	30.55	A
ATOM	822	O	GLN	A	105	82.602	64.258	31.644	1.00	26.07	A
ATOM	823	N	VAL	A	106	83.867	62.889	32.897	1.00	26.33	A

ATOM	824	CA	VAL	A	106	83.888	63.790	34.056	1.00 25.39	A
ATOM	825	CB	VAL	A	106	84.395	63.046	35.315	1.00 24.50	A
ATOM	826	CG1	VAL	A	106	84.635	64.032	36.470	1.00 21.15	A
ATOM	827	CG2	VAL	A	106	83.369	61.966	35.738	1.00 18.61	A
ATOM	828	C	VAL	A	106	84.829	64.931	33.742	1.00 22.14	A
ATOM	829	O	VAL	A	106	84.446	66.083	33.719	1.00 25.05	A
ATOM	830	N	LEU	A	107	86.076	64.589	33.498	1.00 20.26	A
ATOM	831	CA	LEU	A	107	87.076	65.582	33.195	1.00 22.29	A
ATOM	832	CB	LEU	A	107	88.416	64.907	32.888	1.00 19.77	A
ATOM	833	CG	LEU	A	107	89.520	65.924	32.603	1.00 28.38	A
ATOM	834	CD1	LEU	A	107	89.898	66.617	33.883	1.00 29.44	A
ATOM	835	CD2	LEU	A	107	90.737	65.230	32.030	1.00 37.22	A
ATOM	836	C	LEU	A	107	86.652	66.472	32.017	1.00 25.15	A
ATOM	837	O	LEU	A	107	86.572	67.690	32.153	1.00 24.72	A
ATOM	838	N	CYS	A	108	86.334	65.874	30.877	1.00 23.13	A
ATOM	839	CA	CYS	A	108	85.959	66.654	29.711	1.00 20.45	A
ATOM	840	C	CYS	A	108	84.576	67.314	29.811	1.00 27.92	A
ATOM	841	O	CYS	A	108	84.319	68.330	29.156	1.00 25.68	A
ATOM	842	CB	CYS	A	108	86.043	65.787	28.446	1.00 27.49	A
ATOM	843	SG	CYS	A	108	87.690	65.037	28.227	1.00 28.60	A
ATOM	844	N	GLY	A	109	83.684	66.748	30.613	1.00 29.41	A
ATOM	845	CA	GLY	A	109	82.370	67.355	30.765	1.00 21.87	A
ATOM	846	C	GLY	A	109	82.540	68.681	31.483	1.00 26.48	A
ATOM	847	O	GLY	A	109	81.879	69.660	31.155	1.00 24.15	A
ATOM	848	N	ALA	A	110	83.475	68.737	32.440	1.00 19.49	A
ATOM	849	CA	ALA	A	110	83.684	69.970	33.184	1.00 17.06	A
ATOM	850	CB	ALA	A	110	84.578	69.736	34.402	1.00 18.01	A
ATOM	851	C	ALA	A	110	84.318	70.995	32.258	1.00 18.22	A
ATOM	852	O	ALA	A	110	83.970	72.180	32.307	1.00 19.57	A
ATOM	853	N	VAL	A	111	85.268	70.552	31.450	1.00 21.00	A
ATOM	854	CA	VAL	A	111	85.947	71.421	30.492	1.00 19.95	A
ATOM	855	CB	VAL	A	111	87.013	70.609	29.645	1.00 26.47	A
ATOM	856	CG1	VAL	A	111	87.331	71.346	28.314	1.00 19.61	A
ATOM	857	CG2	VAL	A	111	88.307	70.414	30.463	1.00 20.68	A
ATOM	858	C	VAL	A	111	84.883	72.006	29.549	1.00 25.73	A
ATOM	859	O	VAL	A	111	84.835	73.210	29.305	1.00 24.22	A
ATOM	860	N	LYS	A	112	84.016	71.143	29.034	1.00 24.78	A
ATOM	861	CA	LYS	A	112	82.996	71.589	28.096	1.00 29.18	A
ATOM	862	CB	LYS	A	112	82.162	70.391	27.599	1.00 29.48	A
ATOM	863	CG	LYS	A	112	81.141	70.772	26.507	1.00 35.04	A
ATOM	864	CD	LYS	A	112	80.441	69.565	25.878	1.00 35.71	A
ATOM	865	CE	LYS	A	112	81.420	68.677	25.104	1.00 41.21	A
ATOM	866	NZ	LYS	A	112	80.780	67.431	24.529	1.00 43.02	A
ATOM	867	C	LYS	A	112	82.088	72.660	28.688	1.00 24.46	A
ATOM	868	O	LYS	A	112	81.776	73.643	28.024	1.00 26.79	A
ATOM	869	N	TRP	A	113	81.672	72.470	29.939	1.00 23.58	A
ATOM	870	CA	TRP	A	113	80.810	73.415	30.626	1.00 20.72	A
ATOM	871	CB	TRP	A	113	80.459	72.878	32.014	1.00 25.99	A
ATOM	872	CG	TRP	A	113	79.627	73.817	32.856	1.00 22.08	A
ATOM	873	CD2	TRP	A	113	80.101	74.659	33.909	1.00 24.19	A
ATOM	874	CE2	TRP	A	113	78.961	75.282	34.494	1.00 24.99	A
ATOM	875	CE3	TRP	A	113	81.379	74.945	34.426	1.00 19.23	A
ATOM	876	CD1	TRP	A	113	78.251	73.971	32.828	1.00 19.34	A
ATOM	877	NE1	TRP	A	113	77.856	74.845	33.820	1.00 20.42	A
ATOM	878	CZ2	TRP	A	113	79.060	76.153	35.557	1.00 22.43	A

ATOM	879	CZ3	TRP	A	113	81.484	75.808	35.491	1.00	26.60	A
ATOM	880	CH2	TRP	A	113	80.324	76.408	36.056	1.00	30.42	A
ATOM	881	C	TRP	A	113	81.475	74.775	30.793	1.00	23.72	A
ATOM	882	O	TRP	A	113	80.848	75.815	30.600	1.00	21.74	A
ATOM	883	N	LEU	A	114	82.750	74.756	31.182	1.00	23.73	A
ATOM	884	CA	LEU	A	114	83.508	75.976	31.396	1.00	19.99	A
ATOM	885	CB	LEU	A	114	84.971	75.624	31.687	1.00	16.92	A
ATOM	886	CG	LEU	A	114	85.231	75.166	33.138	1.00	17.13	A
ATOM	887	CD1	LEU	A	114	86.620	74.621	33.322	1.00	14.89	A
ATOM	888	CD2	LEU	A	114	85.050	76.365	34.046	1.00	17.43	A
ATOM	889	C	LEU	A	114	83.413	76.839	30.143	1.00	24.77	A
ATOM	890	O	LEU	A	114	83.101	78.042	30.204	1.00	20.50	A
ATOM	891	N	ILE	A	115	83.676	76.197	29.008	1.00	23.02	A
ATOM	892	CA	ILE	A	115	83.670	76.848	27.702	1.00	26.10	A
ATOM	893	CB	ILE	A	115	84.191	75.920	26.552	1.00	24.85	A
ATOM	894	CG2	ILE	A	115	84.215	76.694	25.249	1.00	27.04	A
ATOM	895	CG1	ILE	A	115	85.585	75.368	26.851	1.00	32.98	A
ATOM	896	CD1	ILE	A	115	86.479	76.372	27.492	1.00	52.20	A
ATOM	897	C	ILE	A	115	82.287	77.278	27.240	1.00	23.55	A
ATOM	898	O	ILE	A	115	82.087	78.433	26.884	1.00	21.22	A
ATOM	899	N	LEU	A	116	81.356	76.330	27.222	1.00	15.47	A
ATOM	900	CA	LEU	A	116	80.009	76.584	26.722	1.00	23.51	A
ATOM	901	CB	LEU	A	116	79.298	75.260	26.459	1.00	23.69	A
ATOM	902	CG	LEU	A	116	79.986	74.298	25.494	1.00	29.79	A
ATOM	903	CD1	LEU	A	116	78.985	73.211	25.148	1.00	24.68	A
ATOM	904	CD2	LEU	A	116	80.479	75.022	24.250	1.00	26.74	A
ATOM	905	C	LEU	A	116	79.126	77.454	27.598	1.00	22.96	A
ATOM	906	O	LEU	A	116	78.214	78.095	27.100	1.00	23.54	A
ATOM	907	N	GLU	A	117	79.386	77.479	28.902	1.00	26.63	A
ATOM	908	CA	GLU	A	117	78.567	78.272	29.813	1.00	24.27	A
ATOM	909	CB	GLU	A	117	78.033	77.403	30.936	1.00	21.64	A
ATOM	910	CG	GLU	A	117	77.035	76.355	30.526	1.00	27.37	A
ATOM	911	CD	GLU	A	117	75.767	76.959	29.969	1.00	26.27	A
ATOM	912	OE1	GLU	A	117	75.449	78.124	30.316	1.00	25.92	A
ATOM	913	OE2	GLU	A	117	75.090	76.260	29.191	1.00	30.37	A
ATOM	914	C	GLU	A	117	79.257	79.457	30.470	1.00	24.39	A
ATOM	915	O	GLU	A	117	78.611	80.460	30.753	1.00	25.44	A
ATOM	916	N	LYS	A	118	80.561	79.373	30.706	1.00	18.78	A
ATOM	917	CA	LYS	A	118	81.189	80.460	31.440	1.00	19.49	A
ATOM	918	CB	LYS	A	118	81.782	79.887	32.748	1.00	25.65	A
ATOM	919	CG	LYS	A	118	80.761	79.090	33.606	1.00	17.16	A
ATOM	920	CD	LYS	A	118	79.665	80.070	34.058	1.00	21.32	A
ATOM	921	CE	LYS	A	118	78.463	79.410	34.663	1.00	23.09	A
ATOM	922	NZ	LYS	A	118	77.522	80.476	35.101	1.00	23.88	A
ATOM	923	C	LYS	A	118	82.213	81.332	30.744	1.00	22.37	A
ATOM	924	O	LYS	A	118	82.898	82.122	31.400	1.00	20.49	A
ATOM	925	N	GLN	A	119	82.360	81.262	29.431	1.00	20.57	A
ATOM	926	CA	GLN	A	119	83.332	82.060	28.748	1.00	32.06	A
ATOM	927	CB	GLN	A	119	84.242	81.238	27.801	1.00	20.00	A
ATOM	928	CG	GLN	A	119	85.382	82.091	27.173	1.00	20.89	A
ATOM	929	CD	GLN	A	119	86.339	81.257	26.337	1.00	23.85	A
ATOM	930	OE1	GLN	A	119	85.940	80.270	25.734	1.00	18.93	A
ATOM	931	NE2	GLN	A	119	87.602	81.661	26.285	1.00	15.38	A
ATOM	932	C	GLN	A	119	82.543	83.095	27.929	1.00	24.21	A
ATOM	933	O	GLN	A	119	81.649	82.725	27.195	1.00	21.97	A

ATOM	934	N	LYS	A	120	82.880	84.367	28.048	1.00	28.47	A
ATOM	935	CA	LYS	A	120	82.193	85.403	27.288	1.00	33.91	A
ATOM	936	CB	LYS	A	120	82.448	86.774	27.913	1.00	29.00	A
ATOM	937	CG	LYS	A	120	81.948	86.897	29.337	1.00	38.95	A
ATOM	938	CD	LYS	A	120	82.173	88.303	29.892	1.00	47.54	A
ATOM	939	CE	LYS	A	120	81.955	88.332	31.396	1.00	56.75	A
ATOM	940	NZ	LYS	A	120	80.623	87.776	31.790	1.00	65.69	A
ATOM	941	C	LYS	A	120	82.673	85.434	25.813	1.00	36.89	A
ATOM	942	O	LYS	A	120	83.700	84.864	25.460	1.00	30.22	A
ATOM	943	N	PRO	A	121	81.926	86.120	24.949	1.00	37.55	A
ATOM	944	CD	PRO	A	121	80.622	86.771	25.165	1.00	41.75	A
ATOM	945	CA	PRO	A	121	82.327	86.197	23.548	1.00	31.55	A
ATOM	946	CB	PRO	A	121	81.271	87.114	22.940	1.00	39.82	A
ATOM	947	CG	PRO	A	121	80.041	86.762	23.756	1.00	44.17	A
ATOM	948	C	PRO	A	121	83.724	86.780	23.443	1.00	31.58	A
ATOM	949	O	PRO	A	121	84.489	86.388	22.568	1.00	29.41	A
ATOM	950	N	ASP	A	122	84.076	87.693	24.342	1.00	27.25	A
ATOM	951	CA	ASP	A	122	85.401	88.285	24.268	1.00	29.04	A
ATOM	952	CB	ASP	A	122	85.435	89.636	24.985	1.00	28.38	A
ATOM	953	CG	ASP	A	122	85.281	89.525	26.494	1.00	38.36	A
ATOM	954	OD1	ASP	A	122	84.964	88.438	27.033	1.00	39.09	A
ATOM	955	OD2	ASP	A	122	85.477	90.558	27.156	1.00	38.98	A
ATOM	956	C	ASP	A	122	86.531	87.363	24.733	1.00	32.13	A
ATOM	957	O	ASP	A	122	87.693	87.759	24.780	1.00	25.62	A
ATOM	958	N	GLY	A	123	86.186	86.145	25.214	1.00	30.31	A
ATOM	959	CA	GLY	A	123	87.203	85.196	25.678	1.00	30.38	A
ATOM	960	C	GLY	A	123	87.422	85.098	27.188	1.00	30.19	A
ATOM	961	O	GLY	A	123	88.039	84.144	27.654	1.00	29.94	A
ATOM	962	N	VAL	A	124	86.930	86.077	27.940	1.00	24.05	A
ATOM	963	CA	VAL	A	124	87.055	86.116	29.403	1.00	23.87	A
ATOM	964	CB	VAL	A	124	86.546	87.473	29.951	1.00	23.70	A
ATOM	965	CG1	VAL	A	124	86.353	87.413	31.459	1.00	27.05	A
ATOM	966	CG2	VAL	A	124	87.522	88.581	29.581	1.00	24.79	A
ATOM	967	C	VAL	A	124	86.240	85.041	30.196	1.00	29.58	A
ATOM	968	O	VAL	A	124	85.071	84.813	29.733	1.00	26.81	A
ATOM	969	N	PHE	A	125	86.824	84.383	31.126	1.00	24.92	A
ATOM	970	CA	PHE	A	125	86.040	83.334	31.891	1.00	25.88	A
ATOM	971	CB	PHE	A	125	86.893	82.228	32.350	1.00	24.21	A
ATOM	972	CG	PHE	A	125	87.069	81.189	31.311	1.00	25.00	A
ATOM	973	CD1	PHE	A	125	86.059	80.277	31.059	1.00	23.52	A
ATOM	974	CD2	PHE	A	125	88.224	81.146	30.534	1.00	22.60	A
ATOM	975	CE1	PHE	A	125	86.186	79.345	30.063	1.00	23.68	A
ATOM	976	CE2	PHE	A	125	88.354	80.202	29.517	1.00	16.73	A
ATOM	977	CZ	PHE	A	125	87.338	79.306	29.282	1.00	20.14	A
ATOM	978	C	PHE	A	125	85.479	84.135	33.090	1.00	24.56	A
ATOM	979	O	PHE	A	125	86.175	84.941	33.710	1.00	21.73	A
ATOM	980	N	GLN	A	126	84.214	83.866	33.414	1.00	21.30	A
ATOM	981	CA	GLN	A	126	83.558	84.549	34.539	1.00	22.03	A
ATOM	982	CB	GLN	A	126	82.348	85.333	34.003	1.00	33.53	A
ATOM	983	CG	GLN	A	126	81.694	86.232	35.019	1.00	46.06	A
ATOM	984	CD	GLN	A	126	80.588	87.096	34.409	1.00	54.63	A
ATOM	985	OE1	GLN	A	126	79.474	86.612	34.131	1.00	56.00	A
ATOM	986	NE2	GLN	A	126	80.897	88.383	34.188	1.00	55.55	A
ATOM	987	C	GLN	A	126	83.085	83.607	35.634	1.00	18.80	A
ATOM	988	O	GLN	A	126	82.611	82.489	35.360	1.00	18.84	A

ATOM	989	N	GLU	A	127	83.202	84.068	36.871	1.00 19.63	A
ATOM	990	CA	GLU	A	127	82.770	83.301	38.050	1.00 18.00	A
ATOM	991	CB	GLU	A	127	83.708	83.576	39.232	1.00 17.47	A
ATOM	992	CG	GLU	A	127	83.190	82.969	40.556	1.00 21.51	A
ATOM	993	CD	GLU	A	127	83.051	81.442	40.446	1.00 23.16	A
ATOM	994	OE1	GLU	A	127	82.025	80.930	39.942	1.00 17.83	A
ATOM	995	OE2	GLU	A	127	84.008	80.754	40.848	1.00 21.73	A
ATOM	996	C	GLU	A	127	81.374	83.823	38.419	1.00 26.14	A
ATOM	997	O	GLU	A	127	81.232	85.016	38.663	1.00 21.32	A
ATOM	998	N	ASP	A	128	80.339	82.981	38.438	1.00 24.79	A
ATOM	999	CA	ASP	A	128	79.015	83.486	38.837	1.00 23.86	A
ATOM	1000	CB	ASP	A	128	77.909	83.020	37.876	1.00 28.03	A
ATOM	1001	CG	ASP	A	128	77.970	83.709	36.523	1.00 31.99	A
ATOM	1002	OD1	ASP	A	128	78.166	84.944	36.495	1.00 35.60	A
ATOM	1003	OD2	ASP	A	128	77.807	83.018	35.492	1.00 29.56	A
ATOM	1004	C	ASP	A	128	78.659	83.006	40.253	1.00 20.48	A
ATOM	1005	O	ASP	A	128	77.629	83.368	40.796	1.00 23.11	A
ATOM	1006	N	ALA	A	129	79.498	82.172	40.849	1.00 20.40	A
ATOM	1007	CA	ALA	A	129	79.215	81.676	42.210	1.00 25.25	A
ATOM	1008	CB	ALA	A	129	78.336	80.383	42.153	1.00 24.60	A
ATOM	1009	C	ALA	A	129	80.531	81.385	42.926	1.00 21.47	A
ATOM	1010	O	ALA	A	129	81.012	80.267	42.901	1.00 20.12	A
ATOM	1011	N	PRO	A	130	81.142	82.412	43.535	1.00 22.99	A
ATOM	1012	CD	PRO	A	130	80.707	83.830	43.484	1.00 18.89	A
ATOM	1013	CA	PRO	A	130	82.406	82.269	44.248	1.00 20.89	A
ATOM	1014	CB	PRO	A	130	82.610	83.637	44.868	1.00 24.77	A
ATOM	1015	CG	PRO	A	130	81.951	84.575	43.823	1.00 29.40	A
ATOM	1016	C	PRO	A	130	82.417	81.168	45.314	1.00 25.72	A
ATOM	1017	O	PRO	A	130	81.421	80.932	46.010	1.00 20.76	A
ATOM	1018	N	VAL	A	131	83.557	80.497	45.431	1.00 18.66	A
ATOM	1019	CA	VAL	A	131	83.709	79.442	46.421	1.00 25.11	A
ATOM	1020	CB	VAL	A	131	85.057	78.722	46.307	1.00 15.74	A
ATOM	1021	CG1	VAL	A	131	85.116	77.946	44.960	1.00 15.94	A
ATOM	1022	CG2	VAL	A	131	86.188	79.725	46.459	1.00 19.54	A
ATOM	1023	C	VAL	A	131	83.618	80.030	47.806	1.00 19.19	A
ATOM	1024	O	VAL	A	131	83.848	81.225	48.014	1.00 21.17	A
ATOM	1025	N	ILE	A	132	83.251	79.169	48.747	1.00 18.82	A
ATOM	1026	CA	ILE	A	132	83.149	79.556	50.154	1.00 23.91	A
ATOM	1027	CB	ILE	A	132	82.332	78.512	50.929	1.00 24.37	A
ATOM	1028	CG2	ILE	A	132	82.271	78.876	52.417	1.00 20.00	A
ATOM	1029	CG1	ILE	A	132	80.941	78.425	50.306	1.00 21.42	A
ATOM	1030	CD1	ILE	A	132	80.142	77.180	50.747	1.00 24.98	A
ATOM	1031	C	ILE	A	132	84.541	79.688	50.790	1.00 19.79	A
ATOM	1032	O	ILE	A	132	84.781	80.623	51.520	1.00 17.40	A
ATOM	1033	N	HIS	A	133	85.467	78.766	50.504	1.00 18.82	A
ATOM	1034	CA	HIS	A	133	86.827	78.851	51.100	1.00 17.96	A
ATOM	1035	CB	HIS	A	133	87.434	77.437	51.218	1.00 18.61	A
ATOM	1036	CG	HIS	A	133	86.691	76.548	52.180	1.00 22.75	A
ATOM	1037	CD2	HIS	A	133	85.617	75.738	51.996	1.00 18.28	A
ATOM	1038	ND1	HIS	A	133	86.992	76.499	53.531	1.00 25.58	A
ATOM	1039	CE1	HIS	A	133	86.128	75.693	54.137	1.00 21.42	A
ATOM	1040	NE2	HIS	A	133	85.289	75.222	53.231	1.00 27.04	A
ATOM	1041	C	HIS	A	133	87.711	79.735	50.221	1.00 14.42	A
ATOM	1042	O	HIS	A	133	88.525	79.250	49.431	1.00 17.65	A
ATOM	1043	N	GLN	A	134	87.517	81.039	50.373	1.00 11.52	A

ATOM	1044	CA	GLN	A	134	88.238	82.045	49.608	1.00	21.65	A
ATOM	1045	CB	GLN	A	134	87.689	83.424	50.025	1.00	17.09	A
ATOM	1046	CG	GLN	A	134	86.298	83.729	49.418	1.00	22.43	A
ATOM	1047	CD	GLN	A	134	86.376	84.059	47.908	1.00	21.78	A
ATOM	1048	OE1	GLN	A	134	87.129	84.944	47.522	1.00	28.45	A
ATOM	1049	NE2	GLN	A	134	85.604	83.340	47.061	1.00	22.37	A
ATOM	1050	C	GLN	A	134	89.759	81.873	49.837	1.00	20.34	A
ATOM	1051	O	GLN	A	134	90.565	82.314	49.052	1.00	26.33	A
ATOM	1052	N	GLU	A	135	90.079	81.179	50.928	1.00	19.09	A
ATOM	1053	CA	GLU	A	135	91.407	80.777	51.431	1.00	24.48	A
ATOM	1054	CB	GLU	A	135	91.169	79.850	52.767	1.00	24.93	A
ATOM	1055	CG	GLU	A	135	89.522	79.250	53.099	1.00	4.96	A
ATOM	1056	CD	GLU	A	135	89.446	77.808	53.925	1.00	27.66	A
ATOM	1057	OE1	GLU	A	135	90.527	77.338	53.831	1.00	37.42	A
ATOM	1058	OE2	GLU	A	135	88.528	77.190	54.620	1.00	1.00	A
ATOM	1059	C	GLU	A	135	92.140	79.938	50.318	1.00	20.82	A
ATOM	1060	O	GLU	A	135	93.362	80.014	50.119	1.00	15.84	A
ATOM	1061	N	MET	A	136	91.377	79.109	49.602	1.00	18.40	A
ATOM	1062	CA	MET	A	136	91.967	78.147	48.626	1.00	17.42	A
ATOM	1063	CB	MET	A	136	91.123	76.853	48.571	1.00	15.67	A
ATOM	1064	CG	MET	A	136	89.868	76.961	47.675	1.00	17.99	A
ATOM	1065	SD	MET	A	136	88.703	75.563	47.631	1.00	29.44	A
ATOM	1066	CE	MET	A	136	89.744	74.260	47.009	1.00	11.97	A
ATOM	1067	C	MET	A	136	92.269	78.546	47.203	1.00	15.51	A
ATOM	1068	O	MET	A	136	92.791	77.747	46.443	1.00	14.46	A
ATOM	1069	N	ILE	A	137	91.988	79.787	46.831	1.00	16.94	A
ATOM	1070	CA	ILE	A	137	92.217	80.213	45.449	1.00	15.24	A
ATOM	1071	CB	ILE	A	137	90.980	80.959	44.955	1.00	20.19	A
ATOM	1072	CG2	ILE	A	137	89.724	80.121	45.254	1.00	14.68	A
ATOM	1073	CG1	ILE	A	137	90.847	82.300	45.723	1.00	11.83	A
ATOM	1074	CD1	ILE	A	137	89.473	82.985	45.435	1.00	23.22	A
ATOM	1075	C	ILE	A	137	93.446	81.121	45.287	1.00	19.40	A
ATOM	1076	O	ILE	A	137	93.658	81.729	44.228	1.00	18.10	A
ATOM	1077	N	GLY	A	138	94.222	81.215	46.361	1.00	15.44	A
ATOM	1078	CA	GLY	A	138	95.438	82.007	46.314	1.00	18.65	A
ATOM	1079	C	GLY	A	138	95.197	83.450	45.897	1.00	23.13	A
ATOM	1080	O	GLY	A	138	94.182	84.061	46.313	1.00	15.00	A
ATOM	1081	N	GLY	A	139	96.097	83.962	45.044	1.00	20.15	A
ATOM	1082	CA	GLY	A	139	96.054	85.338	44.585	1.00	17.13	A
ATOM	1083	C	GLY	A	139	94.767	85.808	43.967	1.00	29.17	A
ATOM	1084	O	GLY	A	139	94.568	87.013	43.807	1.00	33.25	A
ATOM	1085	N	LEU	A	140	93.875	84.890	43.618	1.00	23.37	A
ATOM	1086	CA	LEU	A	140	92.621	85.317	43.023	1.00	24.08	A
ATOM	1087	CB	LEU	A	140	91.930	84.142	42.322	1.00	22.29	A
ATOM	1088	CG	LEU	A	140	92.000	84.065	40.800	1.00	36.28	A
ATOM	1089	CD1	LEU	A	140	93.365	84.425	40.297	1.00	39.55	A
ATOM	1090	CD2	LEU	A	140	91.640	82.663	40.376	1.00	31.19	A
ATOM	1091	C	LEU	A	140	91.681	85.918	44.065	1.00	30.45	A
ATOM	1092	O	LEU	A	140	90.698	86.572	43.697	1.00	29.82	A
ATOM	1093	N	ARG	A	141	91.977	85.715	45.353	1.00	23.95	A
ATOM	1094	CA	ARG	A	141	91.105	86.235	46.411	1.00	26.90	A
ATOM	1095	CB	ARG	A	141	91.577	85.782	47.790	1.00	23.51	A
ATOM	1096	CG	ARG	A	141	90.622	86.183	48.883	1.00	31.94	A
ATOM	1097	CD	ARG	A	141	91.045	85.655	50.222	1.00	41.48	A
ATOM	1098	NE	ARG	A	141	90.058	85.983	51.254	1.00	56.61	A

ATOM	1099	CZ	ARG	A	141	89.989	85.390	52.451	1.00	62.59	A
ATOM	1100	NH1	ARG	A	141	90.853	84.427	52.773	1.00	61.70	A
ATOM	1101	NH2	ARG	A	141	89.055	85.761	53.330	1.00	64.29	A
ATOM	1102	C	ARG	A	141	91.103	87.771	46.308	1.00	31.97	A
ATOM	1103	O	ARG	A	141	90.112	88.440	46.571	1.00	35.29	A
ATOM	1104	N	ASN	A	142	92.233	88.327	45.932	1.00	35.39	A
ATOM	1105	CA	ASN	A	142	92.292	89.759	45.708	1.00	47.29	A
ATOM	1106	CB	ASN	A	142	93.755	90.199	45.620	1.00	44.19	A
ATOM	1107	CG	ASN	A	142	93.903	91.672	45.316	1.00	50.84	A
ATOM	1108	OD1	ASN	A	142	93.081	92.260	44.606	1.00	50.20	A
ATOM	1109	ND2	ASN	A	142	94.968	92.273	45.829	1.00	52.23	A
ATOM	1110	C	ASN	A	142	91.588	89.889	44.342	1.00	43.41	A
ATOM	1111	O	ASN	A	142	92.160	89.542	43.302	1.00	41.71	A
ATOM	1112	N	ASN	A	143	90.343	90.361	44.363	1.00	49.05	A
ATOM	1113	CA	ASN	A	143	89.511	90.522	43.151	1.00	54.92	A
ATOM	1114	CB	ASN	A	143	88.071	90.941	43.523	1.00	58.67	A
ATOM	1115	CG	ASN	A	143	87.097	89.762	43.556	1.00	67.74	A
ATOM	1116	OD1	ASN	A	143	87.173	88.843	42.721	1.00	72.16	A
ATOM	1117	ND2	ASN	A	143	86.159	89.795	44.510	1.00	73.35	A
ATOM	1118	C	ASN	A	143	90.024	91.509	42.102	1.00	51.69	A
ATOM	1119	O	ASN	A	143	89.457	91.625	41.012	1.00	52.71	A
ATOM	1120	N	ASN	A	144	91.067	92.245	42.432	1.00	47.25	A
ATOM	1121	CA	ASN	A	144	91.597	93.191	41.479	1.00	47.83	A
ATOM	1122	CB	ASN	A	144	92.706	93.993	42.126	1.00	58.20	A
ATOM	1123	CG	ASN	A	144	92.406	95.451	42.142	1.00	67.49	A
ATOM	1124	OD1	ASN	A	144	92.353	96.070	43.210	1.00	75.34	A
ATOM	1125	ND2	ASN	A	144	92.194	96.027	40.954	1.00	70.42	A
ATOM	1126	C	ASN	A	144	92.157	92.456	40.274	1.00	42.44	A
ATOM	1127	O	ASN	A	144	92.967	91.540	40.432	1.00	43.00	A
ATOM	1128	N	GLU	A	145	91.740	92.866	39.081	1.00	35.72	A
ATOM	1129	CA	GLU	A	145	92.207	92.277	37.832	1.00	30.80	A
ATOM	1130	CB	GLU	A	145	93.751	92.269	37.777	1.00	29.82	A
ATOM	1131	CG	GLU	A	145	94.342	93.705	37.873	1.00	34.98	A
ATOM	1132	CD	GLU	A	145	95.866	93.839	37.711	1.00	33.90	A
ATOM	1133	OE1	GLU	A	145	96.311	94.948	37.366	1.00	37.12	A
ATOM	1134	OE2	GLU	A	145	96.641	92.890	37.938	1.00	36.12	A
ATOM	1135	C	GLU	A	145	91.639	90.883	37.705	1.00	32.53	A
ATOM	1136	O	GLU	A	145	92.261	89.979	37.134	1.00	29.47	A
ATOM	1137	N	LYS	A	146	90.410	90.715	38.179	1.00	33.08	A
ATOM	1138	CA	LYS	A	146	89.809	89.386	38.144	1.00	34.99	A
ATOM	1139	CB	LYS	A	146	88.545	89.324	38.969	1.00	38.84	A
ATOM	1140	CG	LYS	A	146	87.328	89.843	38.309	1.00	46.43	A
ATOM	1141	CD	LYS	A	146	86.173	89.733	39.312	1.00	53.97	A
ATOM	1142	CE	LYS	A	146	84.799	89.902	38.655	1.00	56.22	A
ATOM	1143	NZ	LYS	A	146	84.630	91.185	37.909	1.00	58.13	A
ATOM	1144	C	LYS	A	146	89.597	88.782	36.778	1.00	29.69	A
ATOM	1145	O	LYS	A	146	89.861	87.593	36.608	1.00	22.87	A
ATOM	1146	N	ASP	A	147	89.125	89.558	35.800	1.00	26.03	A
ATOM	1147	CA	ASP	A	147	88.883	88.989	34.459	1.00	24.17	A
ATOM	1148	CB	ASP	A	147	88.363	90.051	33.483	1.00	26.31	A
ATOM	1149	CG	ASP	A	147	86.884	90.374	33.687	1.00	33.37	A
ATOM	1150	OD1	ASP	A	147	86.419	91.396	33.148	1.00	41.72	A
ATOM	1151	OD2	ASP	A	147	86.160	89.619	34.369	1.00	28.33	A
ATOM	1152	C	ASP	A	147	90.175	88.402	33.894	1.00	29.67	A
ATOM	1153	O	ASP	A	147	90.177	87.328	33.291	1.00	30.44	A

ATOM	1154	N	MET	A	148	91.277	89.112	34.087	1.00	21.79	A
ATOM	1155	CA	MET	A	148	92.562	88.631	33.567	1.00	27.79	A
ATOM	1156	CB	MET	A	148	93.591	89.77[illegible]	33.532	1.00	21.45	A
ATOM	1157	CG	MET	A	148	93.406	90.794	32.411	1.00	16.88	A
ATOM	1158	SD	MET	A	148	94.007	90.171	30.836	1.00	26.17	A
ATOM	1159	CE	MET	A	148	95.843	90.114	31.224	1.00	25.36	A
ATOM	1160	C	MET	A	148	93.097	87.46[illegible]	34.431	1.00	23.06	A
ATOM	1161	O	MET	A	148	93.502	86.433	33.902	1.00	26.32	A
ATOM	1162	N	ALA	A	149	93.082	87.630	35.749	1.00	21.95	A
ATOM	1163	CA	ALA	A	149	93.577	86.584	36.637	1.00	26.30	A
ATOM	1164	CB	ALA	A	149	93.539	87.058	38.093	1.00	17.92	A
ATOM	1165	C	ALA	A	149	92.762	85.290	36.464	1.00	24.09	A
ATOM	1166	O	ALA	A	149	93.336	84.239	36.228	1.00	20.02	A
ATOM	1167	N	LEU	A	150	91.441	85.35[illegible]	36.578	1.00	23.60	A
ATOM	1168	CA	LEU	A	150	90.615	84.15[illegible]	36.396	1.00	21.51	A
ATOM	1169	CB	LEU	A	150	89.141	84.431	36.708	1.00	21.03	A
ATOM	1170	CG	LEU	A	150	88.167	83.21[illegible]	36.546	1.00	31.38	A
ATOM	1171	CD1	LEU	A	150	88.557	82.048	37.474	1.00	23.78	A
ATOM	1172	CD2	LEU	A	150	86.725	83.681	36.903	1.00	28.01	A
ATOM	1173	C	LEU	A	150	90.707	83.581	34.985	1.00	26.10	A
ATOM	1174	O	LEU	A	150	90.700	82.351	34.794	1.00	23.93	A
ATOM	1175	N	THR	A	151	90.777	84.442	33.978	1.00	21.82	A
ATOM	1176	CA	THR	A	151	90.895	83.927	32.622	1.00	16.71	A
ATOM	1177	CB	THR	A	151	90.817	85.07[illegible]	31.570	1.00	24.41	A
ATOM	1178	OG1	THR	A	151	89.512	85.68[illegible]	31.646	1.00	24.76	A
ATOM	1179	CG2	THR	A	151	91.004	84.529	30.144	1.00	24.82	A
ATOM	1180	C	THR	A	151	92.199	83.14[illegible]	32.466	1.00	22.41	A
ATOM	1181	O	THR	A	151	92.214	82.09[illegible]	31.853	1.00	22.92	A
ATOM	1182	N	ALA	A	152	93.283	83.633	33.055	1.00	26.27	A
ATOM	1183	CA	ALA	A	152	94.557	82.92[illegible]	32.945	1.00	19.92	A
ATOM	1184	CB	ALA	A	152	95.654	83.75[illegible]	33.543	1.00	15.47	A
ATOM	1185	C	ALA	A	152	94.459	81.57[illegible]	33.671	1.00	19.39	A
ATOM	1186	O	ALA	A	152	94.882	80.56[illegible]	33.133	1.00	19.38	A
ATOM	1187	N	PHE	A	153	93.884	81.603	34.877	1.00	17.38	A
ATOM	1188	CA	PHE	A	153	93.713	80.42[illegible]	35.703	1.00	14.60	A
ATOM	1189	CB	PHE	A	153	92.970	80.71[illegible]	37.004	1.00	17.50	A
ATOM	1190	CG	PHE	A	153	92.773	79.490	37.851	1.00	22.29	A
ATOM	1191	CD1	PHE	A	153	93.813	79.005	38.652	1.00	10.97	A
ATOM	1192	CD2	PHE	A	153	91.551	78.82[illegible]	37.855	1.00	15.16	A
ATOM	1193	CE1	PHE	A	153	93.623	77.853	39.448	1.00	20.47	A
ATOM	1194	CE2	PHE	A	153	91.348	77.68[illegible]	38.636	1.00	22.68	A
ATOM	1195	CZ	PHE	A	153	92.387	77.20[illegible]	39.442	1.00	21.15	A
ATOM	1196	C	PHE	A	153	92.940	79.34[illegible]	34.977	1.00	19.47	A
ATOM	1197	O	PHE	A	153	93.360	78.21[illegible]	34.971	1.00	18.15	A
ATOM	1198	N	VAL	A	154	91.805	79.63[illegible]	34.388	1.00	17.18	A
ATOM	1199	CA	VAL	A	154	91.016	78.66[illegible]	33.662	1.00	14.37	A
ATOM	1200	CB	VAL	A	154	89.598	79.241	33.313	1.00	17.63	A
ATOM	1201	CG1	VAL	A	154	88.830	78.185	32.527	1.00	14.29	A
ATOM	1202	CG2	VAL	A	154	88.835	79.586	34.588	1.00	17.52	A
ATOM	1203	C	VAL	A	154	91.750	78.197	32.416	1.00	19.75	A
ATOM	1204	O	VAL	A	154	91.801	77.003	32.146	1.00	15.15	A
ATOM	1205	N	LEU	A	155	92.336	79.109	31.652	1.00	20.48	A
ATOM	1206	CA	LEU	A	155	93.093	78.710	30.457	1.00	22.98	A
ATOM	1207	CB	LEU	A	155	93.729	79.960	29.791	1.00	16.47	A
ATOM	1208	CG	LEU	A	155	94.688	79.745	28.623	1.00	19.59	A

ATOM	1209	CD1	LEU	A	155	94.015	78.920	27.570	1.00	17.74	A
ATOM	1210	CD2	LEU	A	155	95.164	81.108	28.034	1.00	22.48	A
ATOM	1211	C	LEU	A	155	94.200	77.680	30.800	1.00	16.38	A
ATOM	1212	O	LEU	A	155	94.391	76.711	30.079	1.00	21.06	A
ATOM	1213	N	ILE	A	156	94.926	77.903	31.897	1.00	17.56	A
ATOM	1214	CA	ILE	A	156	96.016	76.992	32.288	1.00	21.21	A
ATOM	1215	CB	ILE	A	156	96.769	77.543	33.538	1.00	23.70	A
ATOM	1216	CG2	ILE	A	156	97.704	76.490	34.155	1.00	17.82	A
ATOM	1217	CG1	ILE	A	156	97.584	78.768	33.108	1.00	20.22	A
ATOM	1218	CD1	ILE	A	156	98.096	79.593	34.297	1.00	15.17	A
ATOM	1219	C	ILE	A	156	95.392	75.608	32.555	1.00	21.00	A
ATOM	1220	O	ILE	A	156	95.955	74.595	32.181	1.00	18.43	A
ATOM	1221	N	SER	A	157	94.222	75.577	33.187	1.00	14.32	A
ATOM	1222	CA	SER	A	157	93.525	74.316	33.425	1.00	22.61	A
ATOM	1223	CB	SER	A	157	92.244	74.564	34.218	1.00	23.22	A
ATOM	1224	OG	SER	A	157	92.563	74.830	35.582	1.00	30.07	A
ATOM	1225	C	SER	A	157	93.174	73.644	32.105	1.00	19.13	A
ATOM	1226	O	SER	A	157	93.405	72.445	31.924	1.00	23.24	A
ATOM	1227	N	LEU	A	158	92.640	74.416	31.163	1.00	23.19	A
ATOM	1228	CA	LEU	A	158	92.268	73.872	29.859	1.00	26.55	A
ATOM	1229	CB	LEU	A	158	91.607	74.955	28.970	1.00	23.19	A
ATOM	1230	CG	LEU	A	158	90.330	75.603	29.537	1.00	28.10	A
ATOM	1231	CD1	LEU	A	158	89.618	76.320	28.444	1.00	30.58	A
ATOM	1232	CD2	LEU	A	158	89.378	74.573	30.117	1.00	26.46	A
ATOM	1233	C	LEU	A	158	93.464	73.293	29.126	1.00	23.77	A
ATOM	1234	O	LEU	A	158	93.342	72.294	28.417	1.00	20.25	A
ATOM	1235	N	GLN	A	159	94.622	73.927	29.269	1.00	20.67	A
ATOM	1236	CA	GLN	A	159	95.823	73.433	28.580	1.00	19.57	A
ATOM	1237	CB	GLN	A	159	96.995	74.418	28.776	1.00	20.64	A
ATOM	1238	CG	GLN	A	159	96.787	75.764	28.118	1.00	25.42	A
ATOM	1239	CD	GLN	A	159	97.003	75.741	26.600	1.00	26.92	A
ATOM	1240	OE1	GLN	A	159	96.865	74.703	25.933	1.00	24.64	A
ATOM	1241	NE2	GLN	A	159	97.341	76.899	26.049	1.00	24.27	A
ATOM	1242	C	GLN	A	159	96.195	72.047	29.136	1.00	25.83	A
ATOM	1243	O	GLN	A	159	96.681	71.182	28.390	1.00	22.57	A
ATOM	1244	N	GLU	A	160	95.963	71.833	30.433	1.00	18.37	A
ATOM	1245	CA	GLU	A	160	96.275	70.533	31.019	1.00	28.44	A
ATOM	1246	CB	GLU	A	160	96.124	70.505	32.537	1.00	18.70	A
ATOM	1247	CG	GLU	A	160	97.204	71.226	33.289	1.00	29.07	A
ATOM	1248	CD	GLU	A	160	97.071	71.010	34.790	1.00	37.12	A
ATOM	1249	OE1	GLU	A	160	96.376	70.046	35.219	1.00	29.05	A
ATOM	1250	OE2	GLU	A	160	97.673	71.806	35.539	1.00	41.97	A
ATOM	1251	C	GLU	A	160	95.364	69.454	30.478	1.00	29.40	A
ATOM	1252	O	GLU	A	160	95.782	68.316	30.357	1.00	24.26	A
ATOM	1253	N	ALA	A	161	94.110	69.796	30.177	1.00	25.80	A
ATOM	1254	CA	ALA	A	161	93.182	68.775	29.705	1.00	26.76	A
ATOM	1255	CB	ALA	A	161	91.827	68.987	30.370	1.00	25.94	A
ATOM	1256	C	ALA	A	161	93.019	68.744	28.193	1.00	29.95	A
ATOM	1257	O	ALA	A	161	92.166	68.029	27.654	1.00	32.80	A
ATOM	1258	N	LYS	A	162	93.848	69.514	27.492	1.00	30.99	A
ATOM	1259	CA	LYS	A	162	93.741	69.628	26.043	1.00	37.27	A
ATOM	1260	CB	LYS	A	162	94.762	70.671	25.557	1.00	38.61	A
ATOM	1261	CG	LYS	A	162	94.792	70.892	24.048	1.00	50.32	A
ATOM	1262	CD	LYS	A	162	95.668	72.093	23.628	1.00	56.78	A
ATOM	1263	CE	LYS	A	162	97.171	71.809	23.618	1.00	58.73	A

ATOM	1264	NZ	LYS	A	162	97.593	70.975	22.433	1.00	57.24	A
ATOM	1265	C	LYS	A	162	93.885	68.321	25.254	1.00	37.81	A
ATOM	1266	O	LYS	A	162	93.029	67.964	24.455	1.00	33.39	A
ATOM	1267	N	ASP	A	163	94.968	67.601	25.475	1.00	41.14	A
ATOM	1268	CA	ASP	A	163	95.171	66.387	24.719	1.00	42.49	A
ATOM	1269	CB	ASP	A	163	96.576	65.858	24.965	1.00	51.70	A
ATOM	1270	CG	ASP	A	163	97.643	66.839	24.512	1.00	57.18	A
ATOM	1271	OD1	ASP	A	163	97.366	67.598	23.557	1.00	62.80	A
ATOM	1272	OD2	ASP	A	163	98.752	66.846	25.094	1.00	64.81	A
ATOM	1273	C	ASP	A	163	94.127	65.361	25.074	1.00	41.86	A
ATOM	1274	O	ASP	A	163	93.582	64.687	24.214	1.00	41.54	A
ATOM	1275	N	ILE	A	164	93.808	65.253	26.344	1.00	37.18	A
ATOM	1276	CA	ILE	A	164	92.801	64.297	26.721	1.00	37.23	A
ATOM	1277	CB	ILE	A	164	92.750	64.158	28.236	1.00	43.08	A
ATOM	1278	CG2	ILE	A	164	91.530	63.365	28.661	1.00	42.32	A
ATOM	1279	CG1	ILE	A	164	94.054	63.514	28.705	1.00	48.60	A
ATOM	1280	CD1	ILE	A	164	94.078	63.174	30.156	1.00	56.10	A
ATOM	1281	C	ILE	A	164	91.404	64.634	26.216	1.00	39.86	A
ATOM	1282	O	ILE	A	164	90.656	63.748	25.830	1.00	33.04	A
ATOM	1283	N	CYS	A	165	91.060	65.914	26.183	1.00	32.76	A
ATOM	1284	CA	CYS	A	165	89.715	66.278	25.814	1.00	34.31	A
ATOM	1285	C	CYS	A	165	89.433	66.817	24.422	1.00	37.19	A
ATOM	1286	O	CYS	A	165	88.287	66.818	24.011	1.00	28.15	A
ATOM	1287	CB	CYS	A	165	89.180	67.278	26.839	1.00	29.46	A
ATOM	1288	SG	CYS	A	165	89.010	66.566	28.503	1.00	28.08	A
ATOM	1289	N	GLU	A	166	90.459	67.264	23.707	1.00	45.15	A
ATOM	1290	CA	GLU	A	166	90.273	67.877	22.395	1.00	51.11	A
ATOM	1291	CB	GLU	A	166	91.630	68.143	21.720	1.00	59.07	A
ATOM	1292	CG	GLU	A	166	92.542	66.935	21.528	1.00	66.72	A
ATOM	1293	CD	GLU	A	166	93.935	67.335	21.000	1.00	71.70	A
ATOM	1294	OE1	GLU	A	166	94.838	66.457	20.967	1.00	74.38	A
ATOM	1295	OE2	GLU	A	166	94.123	68.526	20.619	1.00	68.32	A
ATOM	1296	C	GLU	A	166	89.349	67.152	21.449	1.00	50.97	A
ATOM	1297	O	GLU	A	166	88.661	67.784	20.646	1.00	50.00	A
ATOM	1298	N	GLU	A	167	89.314	65.833	21.559	1.00	52.19	A
ATOM	1299	CA	GLU	A	167	88.448	65.027	20.718	1.00	52.32	A
ATOM	1300	CB	GLU	A	167	88.840	63.559	20.838	1.00	50.45	A
ATOM	1301	CG	GLU	A	167	89.074	62.885	19.504	1.00	68.41	A
ATOM	1302	CD	GLU	A	167	89.979	63.713	18.605	1.00	74.42	A
ATOM	1303	OE1	GLU	A	167	91.048	64.161	19.082	1.00	77.67	A
ATOM	1304	OE2	GLU	A	167	89.621	63.917	17.421	1.00	78.62	A
ATOM	1305	C	GLU	A	167	86.963	65.177	21.059	1.00	54.06	A
ATOM	1306	O	GLU	A	167	86.136	65.356	20.163	1.00	52.37	A
ATOM	1307	N	GLN	A	168	86.632	65.103	22.351	1.00	46.71	A
ATOM	1308	CA	GLN	A	168	85.247	65.202	22.811	1.00	43.91	A
ATOM	1309	CB	GLN	A	168	85.059	64.480	24.155	1.00	50.94	A
ATOM	1310	CG	GLN	A	168	86.269	64.533	25.087	1.00	56.41	A
ATOM	1311	CD	GLN	A	168	87.154	63.284	24.976	1.00	55.96	A
ATOM	1312	OE1	GLN	A	168	86.830	62.226	25.526	1.00	49.92	A
ATOM	1313	NE2	GLN	A	168	88.268	63.406	24.247	1.00	57.62	A
ATOM	1314	C	GLN	A	168	84.752	66.620	22.959	1.00	42.37	A
ATOM	1315	O	GLN	A	168	83.547	66.856	23.073	1.00	41.71	A
ATOM	1316	N	VAL	A	169	85.673	67.571	22.965	1.00	33.31	A
ATOM	1317	CA	VAL	A	169	85.281	68.962	23.112	1.00	35.06	A
ATOM	1318	CB	VAL	A	169	85.809	69.506	24.469	1.00	27.42	A

ATOM	1319	CG1	VAL	A	169	85.245	70.889	24.754	1.00	25.13	A
ATOM	1320	CG2	VAL	A	169	85.402	68.540	25.573	1.00	24.56	A
ATOM	1321	C	VAL	A	169	85.780	69.792	21.919	1.00	34.13	A
ATOM	1322	O	VAL	A	169	86.866	70.376	21.962	1.00	31.73	A
ATOM	1323	N	ASN	A	170	84.971	69.841	20.857	1.00	31.12	A
ATOM	1324	CA	ASN	A	170	85.367	70.554	19.646	1.00	31.56	A
ATOM	1325	CB	ASN	A	170	84.377	70.283	18.503	1.00	38.49	A
ATOM	1326	CG	ASN	A	170	84.352	68.798	18.058	1.00	44.51	A
ATOM	1327	OD1	ASN	A	170	83.419	68.063	18.367	1.00	50.11	A
ATOM	1328	ND2	ASN	A	170	85.374	68.375	17.334	1.00	40.85	A
ATOM	1329	C	ASN	A	170	85.562	72.052	19.838	1.00	33.38	A
ATOM	1330	O	ASN	A	170	86.308	72.682	19.101	1.00	32.60	A
ATOM	1331	N	SER	A	171	84.931	72.641	20.843	1.00	29.65	A
ATOM	1332	CA	SER	A	171	85.123	74.080	21.054	1.00	27.07	A
ATOM	1333	CB	SER	A	171	83.937	74.650	21.858	1.00	26.83	A
ATOM	1334	OG	SER	A	171	83.675	73.861	23.020	1.00	22.03	A
ATOM	1335	C	SER	A	171	86.434	74.410	21.776	1.00	23.40	A
ATOM	1336	O	SER	A	171	86.829	75.571	21.868	1.00	25.17	A
ATOM	1337	N	LEU	A	172	87.130	73.400	22.274	1.00	20.64	A
ATOM	1338	CA	LEU	A	172	88.364	73.670	23.024	1.00	18.28	A
ATOM	1339	CB	LEU	A	172	88.976	72.340	23.451	1.00	26.95	A
ATOM	1340	CG	LEU	A	172	89.987	72.252	24.605	1.00	36.59	A
ATOM	1341	CD1	LEU	A	172	89.724	73.283	25.714	1.00	28.04	A
ATOM	1342	CD2	LEU	A	172	89.912	70.840	25.159	1.00	30.83	A
ATOM	1343	C	LEU	A	172	89.420	74.540	22.325	1.00	23.79	A
ATOM	1344	O	LEU	A	172	89.867	75.551	22.863	1.00	22.52	A
ATOM	1345	N	PRO	A	173	89.821	74.173	21.095	1.00	28.78	A
ATOM	1346	CD	PRO	A	173	89.392	73.036	20.258	1.00	26.81	A
ATOM	1347	CA	PRO	A	173	90.837	74.991	20.419	1.00	28.96	A
ATOM	1348	CB	PRO	A	173	91.001	74.308	19.054	1.00	28.65	A
ATOM	1349	CG	PRO	A	173	90.597	72.878	19.321	1.00	33.10	A
ATOM	1350	C	PRO	A	173	90.454	76.475	20.301	1.00	27.14	A
ATOM	1351	O	PRO	A	173	91.259	77.366	20.599	1.00	22.88	A
ATOM	1352	N	GLY	A	174	89.223	76.730	19.885	1.00	24.04	A
ATOM	1353	CA	GLY	A	174	88.771	78.104	19.731	1.00	24.51	A
ATOM	1354	C	GLY	A	174	88.067	78.805	21.071	1.00	23.82	A
ATOM	1355	O	GLY	A	174	88.943	79.985	21.172	1.00	24.00	A
ATOM	1356	N	SER	A	175	88.269	78.083	22.115	1.00	23.65	A
ATOM	1357	CA	SER	A	175	88.167	78.706	23.462	1.00	25.41	A
ATOM	1358	CB	SER	A	175	87.662	77.665	24.489	1.00	21.04	A
ATOM	1359	OG	SER	A	175	87.648	78.213	25.791	1.00	22.86	A
ATOM	1360	C	SER	A	175	89.534	79.224	23.917	1.00	23.64	A
ATOM	1361	O	SER	A	175	89.691	80.347	24.440	1.00	21.39	A
ATOM	1362	N	ILE	A	176	90.531	78.372	23.741	1.00	24.52	A
ATOM	1363	CA	ILE	A	176	91.907	78.683	24.127	1.00	20.94	A
ATOM	1364	CB	ILE	A	176	92.774	77.406	23.873	1.00	19.98	A
ATOM	1365	CG2	ILE	A	176	91.244	77.741	23.797	1.00	20.82	A
ATOM	1366	CG1	ILE	A	176	92.449	76.370	24.970	1.00	23.34	A
ATOM	1367	CD1	ILE	A	176	93.191	75.017	24.797	1.00	23.21	A
ATOM	1368	C	ILE	A	176	92.427	79.921	23.371	1.00	23.29	A
ATOM	1369	O	ILE	A	176	93.011	80.845	23.953	1.00	21.00	A
ATOM	1370	N	THR	A	177	92.180	79.957	22.069	1.00	22.38	A
ATOM	1371	CA	THR	A	177	92.622	81.096	21.280	1.00	26.70	A
ATOM	1372	CB	THR	A	177	92.298	80.826	19.810	1.00	30.44	A
ATOM	1373	OG1	THR	A	177	93.142	79.754	19.352	1.00	32.66	A

ATOM	1374	CG2	THR	A	177	92.507	82.071	18.959	1.00	25.97	A
ATOM	1375	C	THR	A	177	92.966	82.395	21.793	1.00	28.53	A
ATOM	1376	O	THR	A	177	92.635	83.437	21.992	1.00	25.08	A
ATOM	1377	N	LYS	A	178	90.665	82.320	22.058	1.00	24.69	A
ATOM	1378	CA	LYS	A	178	89.966	83.486	22.556	1.00	22.85	A
ATOM	1379	CB	LYS	A	178	88.458	83.212	22.647	1.00	33.69	A
ATOM	1380	CG	LYS	A	178	87.719	83.233	21.285	1.00	37.81	A
ATOM	1381	CD	LYS	A	178	86.260	82.880	21.478	1.00	45.50	A
ATOM	1382	CE	LYS	A	178	85.580	82.539	20.168	1.00	55.66	A
ATOM	1383	NZ	LYS	A	178	84.321	81.738	20.375	1.00	62.92	A
ATOM	1384	C	LYS	A	178	90.513	83.903	23.908	1.00	27.56	A
ATOM	1385	O	LYS	A	178	90.764	85.100	24.139	1.00	22.42	A
ATOM	1386	N	ALA	A	179	90.708	82.945	24.818	1.00	21.82	A
ATOM	1387	CA	ALA	A	179	91.232	83.327	26.117	1.00	22.17	A
ATOM	1388	CB	ALA	A	179	91.326	82.107	27.056	1.00	20.58	A
ATOM	1389	C	ALA	A	179	92.607	83.918	25.879	1.00	23.19	A
ATOM	1390	O	ALA	A	179	92.958	84.970	26.424	1.00	21.73	A
ATOM	1391	N	GLY	A	180	93.392	83.244	25.046	1.00	26.28	A
ATOM	1392	CA	GLY	A	180	94.732	83.741	24.790	1.00	25.77	A
ATOM	1393	C	GLY	A	180	94.723	85.155	24.206	1.00	29.69	A
ATOM	1394	O	GLY	A	180	95.509	86.005	24.628	1.00	26.61	A
ATOM	1395	N	ASP	A	181	93.869	85.403	23.215	1.00	19.22	A
ATOM	1396	CA	ASP	A	181	93.776	86.745	22.600	1.00	24.71	A
ATOM	1397	CB	ASP	A	181	92.670	86.781	21.544	1.00	28.40	A
ATOM	1398	CG	ASP	A	181	93.045	86.061	20.266	1.00	24.26	A
ATOM	1399	OD1	ASP	A	181	94.242	85.821	20.035	1.00	26.47	A
ATOM	1400	OD2	ASP	A	181	92.138	85.751	19.475	1.00	31.29	A
ATOM	1401	C	ASP	A	181	93.465	87.814	23.635	1.00	23.38	A
ATOM	1402	O	ASP	A	181	94.051	88.897	23.619	1.00	24.92	A
ATOM	1403	N	PHE	A	182	92.541	87.508	24.548	1.00	23.93	A
ATOM	1404	CA	PHE	A	182	92.179	88.481	25.562	1.00	24.17	A
ATOM	1405	CB	PHE	A	182	90.971	88.008	26.368	1.00	29.71	A
ATOM	1406	CG	PHE	A	182	90.573	88.970	27.457	1.00	37.61	A
ATOM	1407	CD1	PHE	A	182	89.777	90.074	27.174	1.00	35.83	A
ATOM	1408	CD2	PHE	A	182	91.034	88.798	28.751	1.00	37.07	A
ATOM	1409	CE1	PHE	A	182	89.447	90.989	28.165	1.00	38.94	A
ATOM	1410	CE2	PHE	A	182	90.706	89.712	29.748	1.00	42.65	A
ATOM	1411	CZ	PHE	A	182	89.915	90.806	29.456	1.00	41.10	A
ATOM	1412	C	PHE	A	182	93.343	88.759	26.514	1.00	29.73	A
ATOM	1413	O	PHE	A	182	93.610	89.911	26.877	1.00	26.64	A
ATOM	1414	N	LEU	A	183	94.041	87.710	26.933	1.00	23.11	A
ATOM	1415	CA	LEU	A	183	95.163	87.923	27.847	1.00	23.03	A
ATOM	1416	CB	LEU	A	183	95.794	86.587	28.302	1.00	19.13	A
ATOM	1417	CG	LEU	A	183	94.927	85.684	29.181	1.00	24.04	A
ATOM	1418	CD1	LEU	A	183	95.697	84.363	29.487	1.00	23.39	A
ATOM	1419	CD2	LEU	A	183	94.595	86.398	30.489	1.00	21.06	A
ATOM	1420	C	LEU	A	183	96.237	88.742	27.140	1.00	19.58	A
ATOM	1421	O	LEU	A	183	96.797	89.668	27.721	1.00	23.81	A
ATOM	1422	N	GLU	A	184	96.545	88.383	25.904	1.00	19.16	A
ATOM	1423	CA	GLU	A	184	97.584	89.114	25.190	1.00	29.47	A
ATOM	1424	CB	GLU	A	184	97.874	88.459	23.842	1.00	27.07	A
ATOM	1425	CG	GLU	A	184	98.874	89.217	23.010	1.00	33.26	A
ATOM	1426	CD	GLU	A	184	99.360	88.416	21.817	1.00	36.59	A
ATOM	1427	OE1	GLU	A	184	98.869	87.295	21.569	1.00	37.18	A
ATOM	1428	OE2	GLU	A	184	100.249	88.907	21.120	1.00	40.45	A

ATOM	1429	C	GLU	A	184	97.204	90.578	24.992	1.00	26.03	A
ATOM	1430	O	GLU	A	184	98.004	91.471	25.273	1.00	29.51	A
ATOM	1431	N	ALA	A	185	95.981	90.835	24.548	1.00	28.37	A
ATOM	1432	CA	ALA	A	185	95.560	92.236	24.317	1.00	32.04	A
ATOM	1433	CB	ALA	A	185	94.166	92.282	23.689	1.00	31.81	A
ATOM	1434	C	ALA	A	185	95.567	93.137	25.537	1.00	36.13	A
ATOM	1435	O	ALA	A	185	95.706	94.353	25.401	1.00	35.39	A
ATOM	1436	N	ASN	A	186	95.448	92.555	26.730	1.00	32.84	A
ATOM	1437	CA	ASN	A	186	95.352	93.351	27.953	1.00	29.26	A
ATOM	1438	CB	ASN	A	186	94.035	93.004	28.640	1.00	27.88	A
ATOM	1439	CG	ASN	A	186	92.847	93.480	27.836	1.00	33.22	A
ATOM	1440	OD1	ASN	A	186	92.562	94.672	27.813	1.00	34.12	A
ATOM	1441	ND2	ASN	A	186	92.175	92.566	27.143	1.00	25.25	A
ATOM	1442	C	ASN	A	186	96.476	93.240	28.952	1.00	27.19	A
ATOM	1443	O	ASN	A	186	96.444	93.890	30.003	1.00	27.97	A
ATOM	1444	N	TYR	A	187	97.472	92.433	28.610	1.00	24.51	A
ATOM	1445	CA	TYR	A	187	98.612	92.176	29.486	1.00	21.48	A
ATOM	1446	CB	TYR	A	187	99.634	91.255	28.785	1.00	23.19	A
ATOM	1447	CG	TYR	A	187	100.651	90.604	29.729	1.00	27.39	A
ATOM	1448	CD1	TYR	A	187	100.258	89.596	30.637	1.00	24.03	A
ATOM	1449	CE1	TYR	A	187	101.209	88.977	31.508	1.00	28.63	A
ATOM	1450	CD2	TYR	A	187	102.004	90.982	29.712	1.00	25.92	A
ATOM	1451	CE2	TYR	A	187	102.952	90.380	30.570	1.00	28.97	A
ATOM	1452	CZ	TYR	A	187	102.551	89.379	31.465	1.00	31.32	A
ATOM	1453	OH	TYR	A	187	103.498	88.738	32.293	1.00	25.25	A
ATOM	1454	C	TYR	A	187	99.360	93.389	29.929	1.00	29.36	A
ATOM	1455	O	TYR	A	187	99.645	93.536	31.122	1.00	26.96	A
ATOM	1456	N	MET	A	188	99.721	94.240	28.956	1.00	25.41	A
ATOM	1457	CA	MET	A	188	100.526	95.417	29.260	1.00	31.50	A
ATOM	1458	CB	MET	A	188	100.794	96.215	27.981	1.00	24.85	A
ATOM	1459	CG	MET	A	188	101.699	95.478	27.011	1.00	26.87	A
ATOM	1460	SD	MET	A	188	103.259	94.935	27.730	1.00	33.34	A
ATOM	1461	CE	MET	A	188	103.886	96.512	28.315	1.00	30.68	A
ATOM	1462	C	MET	A	188	99.967	96.322	30.349	1.00	27.28	A
ATOM	1463	O	MET	A	188	100.720	96.982	31.071	1.00	26.43	A
ATOM	1464	N	ASN	A	189	98.645	96.288	30.495	1.00	25.67	A
ATOM	1465	CA	ASN	A	189	97.927	97.092	31.482	1.00	40.32	A
ATOM	1466	CB	ASN	A	189	96.439	97.323	31.000	1.00	46.12	A
ATOM	1467	CG	ASN	A	189	96.220	98.769	30.729	1.00	58.01	A
ATOM	1468	OD1	ASN	A	189	95.564	99.113	29.728	1.00	63.96	A
ATOM	1469	ND2	ASN	A	189	96.722	99.643	31.612	1.00	54.68	A
ATOM	1470	C	ASN	A	189	97.850	96.519	32.897	1.00	40.44	A
ATOM	1471	O	ASN	A	189	97.220	97.109	33.770	1.00	40.07	A
ATOM	1472	N	LEU	A	190	98.469	95.375	33.140	1.00	37.09	A
ATOM	1473	CA	LEU	A	190	98.391	94.795	34.473	1.00	32.05	A
ATOM	1474	CB	LEU	A	190	98.887	93.358	34.459	1.00	27.91	A
ATOM	1475	CG	LEU	A	190	98.000	92.410	33.659	1.00	25.90	A
ATOM	1476	CD1	LEU	A	190	98.707	91.036	33.591	1.00	21.96	A
ATOM	1477	CD2	LEU	A	190	96.619	92.343	34.315	1.00	19.68	A
ATOM	1478	C	LEU	A	190	99.186	95.549	35.485	1.00	32.08	A
ATOM	1479	O	LEU	A	190	100.264	96.039	35.189	1.00	34.79	A
ATOM	1480	N	GLN	A	191	98.653	95.630	36.696	1.00	24.96	A
ATOM	1481	CA	GLN	A	191	99.359	96.299	37.771	1.00	29.96	A
ATOM	1482	CB	GLN	A	191	98.443	97.330	38.429	1.00	37.43	A
ATOM	1483	CG	GLN	A	191	98.000	98.434	37.486	1.00	50.78	A

ATOM	1484	CD	GLN	A	191	99.178	99.289	37.084	1.00	58.93	A
ATOM	1485	OE1	GLN	A	191	99.756	99.994	37.923	1.00	65.09	A
ATOM	1486	NE2	GLN	A	191	99.566	99.220	35.803	1.00	65.13	A
ATOM	1487	C	GLN	A	191	99.878	95.333	38.855	1.00	32.15	A
ATOM	1488	O	GLN	A	191	100.893	95.610	39.464	1.00	28.48	A
ATOM	1489	N	ARG	A	192	99.189	94.219	39.119	1.00	25.14	A
ATOM	1490	CA	ARG	A	192	99.657	93.312	40.170	1.00	22.86	A
ATOM	1491	CB	ARG	A	192	98.489	92.473	40.703	1.00	23.64	A
ATOM	1492	CG	ARG	A	192	97.302	93.308	41.257	1.00	31.91	A
ATOM	1493	CD	ARG	A	192	96.128	92.393	41.622	1.00	35.16	A
ATOM	1494	NE	ARG	A	192	96.514	91.335	42.569	1.00	41.51	A
ATOM	1495	CZ	ARG	A	192	95.847	90.184	42.733	1.00	44.28	A
ATOM	1496	NH1	ARG	A	192	94.757	89.949	41.997	1.00	39.94	A
ATOM	1497	NH2	ARG	A	192	96.255	89.280	43.641	1.00	30.46	A
ATOM	1498	C	ARG	A	192	100.736	92.356	39.709	1.00	19.29	A
ATOM	1499	O	ARG	A	192	100.658	91.822	38.596	1.00	15.56	A
ATOM	1500	N	SER	A	193	101.735	92.114	40.557	1.00	20.51	A
ATOM	1501	CA	SER	A	193	102.769	91.138	40.196	1.00	23.99	A
ATOM	1502	CB	SER	A	193	103.853	91.066	41.250	1.00	25.82	A
ATOM	1503	OG	SER	A	193	104.634	92.236	41.177	1.00	29.45	A
ATOM	1504	C	SER	A	193	102.123	89.754	40.041	1.00	26.36	A
ATOM	1505	O	SER	A	193	102.508	88.958	39.164	1.00	26.52	A
ATOM	1506	N	TYR	A	194	101.123	89.479	40.877	1.00	27.26	A
ATOM	1507	CA	TYR	A	194	100.429	88.201	40.790	1.00	22.13	A
ATOM	1508	CB	TYR	A	194	99.303	88.108	41.823	1.00	23.41	A
ATOM	1509	CG	TYR	A	194	98.539	86.783	41.755	1.00	16.74	A
ATOM	1510	CD1	TYR	A	194	99.067	85.620	42.340	1.00	19.51	A
ATOM	1511	CE1	TYR	A	194	98.401	84.389	42.271	1.00	17.85	A
ATOM	1512	CD2	TYR	A	194	97.312	86.692	41.087	1.00	20.75	A
ATOM	1513	CE2	TYR	A	194	96.621	85.461	41.001	1.00	25.88	A
ATOM	1514	CZ	TYR	A	194	97.181	84.312	41.603	1.00	20.62	A
ATOM	1515	OH	TYR	A	194	96.522	83.107	41.540	1.00	24.87	A
ATOM	1516	C	TYR	A	194	99.843	87.964	39.398	1.00	23.17	A
ATOM	1517	O	TYR	A	194	100.123	86.948	38.775	1.00	22.83	A
ATOM	1518	N	THR	A	195	99.013	88.878	38.904	1.00	18.74	A
ATOM	1519	CA	THR	A	195	98.391	88.680	37.602	1.00	16.68	A
ATOM	1520	CB	THR	A	195	97.427	89.817	37.264	1.00	16.43	A
ATOM	1521	OG1	THR	A	195	96.657	90.130	38.428	1.00	21.65	A
ATOM	1522	CG2	THR	A	195	96.496	89.378	36.151	1.00	22.25	A
ATOM	1523	C	THR	A	195	99.437	88.593	36.498	1.00	21.37	A
ATOM	1524	O	THR	A	195	99.315	87.829	35.549	1.00	18.17	A
ATOM	1525	N	VAL	A	196	100.506	89.359	36.647	1.00	23.63	A
ATOM	1526	CA	VAL	A	196	101.531	89.334	35.639	1.00	20.64	A
ATOM	1527	CB	VAL	A	196	102.620	90.409	35.959	1.00	26.84	A
ATOM	1528	CG1	VAL	A	196	103.973	90.045	35.324	1.00	25.77	A
ATOM	1529	CG2	VAL	A	196	102.154	91.773	35.456	1.00	25.74	A
ATOM	1530	C	VAL	A	196	102.147	87.933	35.583	1.00	20.37	A
ATOM	1531	O	VAL	A	196	102.451	87.439	34.503	1.00	19.78	A
ATOM	1532	N	ALA	A	197	102.386	87.326	36.739	1.00	21.05	A
ATOM	1533	CA	ALA	A	197	103.005	85.984	36.766	1.00	24.45	A
ATOM	1534	CB	ALA	A	197	103.370	85.583	38.225	1.00	15.17	A
ATOM	1535	C	ALA	A	197	102.056	84.951	36.162	1.00	15.00	A
ATOM	1536	O	ALA	A	197	102.424	84.229	35.226	1.00	20.20	A
ATOM	1537	N	ILE	A	198	100.809	84.911	36.648	1.00	24.78	A
ATOM	1538	CA	ILE	A	198	99.887	83.889	36.144	1.00	20.75	A

ATOM	1539	CB	ILE	A	198	98.569	83.723	37.056	1.00	19.12	A
ATOM	1540	CG2	ILE	A	198	97.602	84.931	36.915	1.00	20.52	A
ATOM	1541	CG1	ILE	A	198	97.855	82.438	36.658	1.00	19.50	A
ATOM	1542	CD1	ILE	A	198	96.670	82.071	37.553	1.00	20.96	A
ATOM	1543	C	ILE	A	198	99.545	84.052	34.674	1.00	19.83	A
ATOM	1544	O	ILE	A	198	99.593	83.057	33.913	1.00	21.51	A
ATOM	1545	N	ALA	A	199	99.217	85.274	34.235	1.00	19.78	A
ATOM	1546	CA	ALA	A	199	98.921	85.448	32.814	1.00	19.70	A
ATOM	1547	CB	ALA	A	199	98.323	86.823	32.537	1.00	18.52	A
ATOM	1548	C	ALA	A	199	100.226	85.268	32.049	1.00	11.15	A
ATOM	1549	O	ALA	A	199	100.228	84.804	30.911	1.00	17.30	A
ATOM	1550	N	GLY	A	200	101.345	85.621	32.680	1.00	17.10	A
ATOM	1551	CA	GLY	A	200	102.617	85.447	32.002	1.00	19.39	A
ATOM	1552	C	GLY	A	200	102.800	83.976	31.647	1.00	21.92	A
ATOM	1553	O	GLY	A	200	103.113	83.615	30.486	1.00	19.30	A
ATOM	1554	N	TYR	A	201	102.578	83.097	32.628	1.00	17.66	A
ATOM	1555	CA	TYR	A	201	102.742	81.670	32.329	1.00	23.38	A
ATOM	1556	CB	TYR	A	201	102.550	80.804	33.587	1.00	17.53	A
ATOM	1557	CG	TYR	A	201	102.641	79.303	33.313	1.00	19.35	A
ATOM	1558	CD1	TYR	A	201	103.714	78.768	32.608	1.00	20.15	A
ATOM	1559	CE1	TYR	A	201	103.815	77.383	32.384	1.00	25.42	A
ATOM	1560	CD2	TYR	A	201	101.663	78.420	33.788	1.00	26.23	A
ATOM	1561	CE2	TYR	A	201	101.749	77.037	33.573	1.00	17.93	A
ATOM	1562	CZ	TYR	A	201	102.816	76.528	32.883	1.00	25.37	A
ATOM	1563	OH	TYR	A	201	102.908	75.171	32.690	1.00	24.20	A
ATOM	1564	C	TYR	A	201	101.740	81.238	31.242	1.00	23.90	A
ATOM	1565	O	TYR	A	201	102.098	80.503	30.312	1.00	18.43	A
ATOM	1566	N	ALA	A	202	100.490	81.698	31.349	1.00	19.10	A
ATOM	1567	CA	ALA	A	202	99.484	81.306	30.367	1.00	22.19	A
ATOM	1568	CB	ALA	A	202	98.132	81.940	30.715	1.00	19.48	A
ATOM	1569	C	ALA	A	202	99.916	81.720	28.963	1.00	23.29	A
ATOM	1570	O	ALA	A	202	99.730	80.969	28.004	1.00	23.99	A
ATOM	1571	N	LEU	A	203	100.487	82.919	28.832	1.00	23.24	A
ATOM	1572	CA	LEU	A	203	100.929	83.371	27.510	1.00	23.06	A
ATOM	1573	CB	LEU	A	203	101.178	84.894	27.514	1.00	24.75	A
ATOM	1574	CG	LEU	A	203	99.907	85.744	27.664	1.00	23.34	A
ATOM	1575	CD1	LEU	A	203	100.306	87.220	27.773	1.00	27.91	A
ATOM	1576	CD2	LEU	A	203	98.963	85.548	26.489	1.00	21.31	A
ATOM	1577	C	LEU	A	203	102.182	82.611	27.060	1.00	20.01	A
ATOM	1578	O	LEU	A	203	102.321	82.260	25.892	1.00	22.51	A
ATOM	1579	N	ALA	A	204	103.087	82.325	27.985	1.00	20.31	A
ATOM	1580	CA	ALA	A	204	104.291	81.588	27.615	1.00	19.81	A
ATOM	1581	CB	ALA	A	204	105.193	81.391	28.819	1.00	16.54	A
ATOM	1582	C	ALA	A	204	103.893	80.248	27.035	1.00	22.33	A
ATOM	1583	O	ALA	A	204	104.477	79.812	26.060	1.00	23.53	A
ATOM	1584	N	GLN	A	205	102.881	79.588	27.607	1.00	21.05	A
ATOM	1585	CA	GLN	A	205	102.483	78.289	27.059	1.00	21.95	A
ATOM	1586	CB	GLN	A	205	101.309	77.717	27.840	1.00	18.19	A
ATOM	1587	CG	GLN	A	205	101.588	77.415	29.314	1.00	25.79	A
ATOM	1588	CD	GLN	A	205	100.431	76.681	29.929	1.00	29.43	A
ATOM	1589	OE1	GLN	A	205	99.299	77.200	29.967	1.00	23.15	A
ATOM	1590	NE2	GLN	A	205	100.685	75.451	30.399	1.00	23.34	A
ATOM	1591	C	GLN	A	205	102.068	78.366	25.586	1.00	27.79	A
ATOM	1592	O	GLN	A	205	102.165	77.392	24.847	1.00	24.19	A
ATOM	1593	N	MET	A	206	101.575	79.525	25.164	1.00	26.44	A

ATOM	1594	CA	MET	A	206	101.117	79.661	23.789	1.00 29.37	A
ATOM	1595	CB	MET	A	206	99.802	80.452	23.771	1.00 26.17	A
ATOM	1596	CG	MET	A	206	98.806	80.012	24.828	1.00 30.40	A
ATOM	1597	SD	MET	A	206	97.200	80.847	24.728	1.00 29.96	A
ATOM	1598	CE	MET	A	206	97.598	82.319	25.513	1.00 41.60	A
ATOM	1599	C	MET	A	206	102.138	80.349	22.889	1.00 29.92	A
ATOM	1600	O	MET	A	206	101.828	80.674	21.749	1.00 26.65	A
ATOM	1601	N	GLY	A	207	103.345	80.586	23.394	1.00 29.43	A
ATOM	1602	CA	GLY	A	207	104.352	81.278	22.593	1.00 26.83	A
ATOM	1603	C	GLY	A	207	104.014	82.753	22.378	1.00 34.90	A
ATOM	1604	O	GLY	A	207	104.534	83.393	21.464	1.00 27.87	A
ATOM	1605	N	ARG	A	208	103.171	83.313	23.244	1.00 27.86	A
ATOM	1606	CA	ARG	A	208	102.784	84.698	23.207	1.00 34.19	A
ATOM	1607	CB	ARG	A	208	101.256	84.788	23.147	1.00 33.23	A
ATOM	1608	CG	ARG	A	208	100.654	84.008	21.992	1.00 38.52	A
ATOM	1609	CD	ARG	A	208	99.191	83.574	22.162	1.00 42.22	A
ATOM	1610	NE	ARG	A	208	98.288	84.690	21.974	1.00 49.84	A
ATOM	1611	CZ	ARG	A	208	97.110	84.638	21.362	1.00 42.43	A
ATOM	1612	NH1	ARG	A	208	96.641	83.509	20.856	1.00 38.92	A
ATOM	1613	NH2	ARG	A	208	96.416	85.753	21.233	1.00 48.94	A
ATOM	1614	C	ARG	A	208	103.430	85.669	24.080	1.00 32.61	A
ATOM	1615	O	ARG	A	208	103.113	86.839	24.056	1.00 31.15	A
ATOM	1616	N	LEU	A	209	104.333	85.197	24.934	1.00 26.57	A
ATOM	1617	CA	LEU	A	209	104.990	86.093	25.879	1.00 31.14	A
ATOM	1618	CB	LEU	A	209	105.271	85.369	27.211	1.00 22.61	A
ATOM	1619	CG	LEU	A	209	105.798	86.228	28.366	1.00 35.65	A
ATOM	1620	CD1	LEU	A	209	104.766	87.332	28.723	1.00 28.29	A
ATOM	1621	CD2	LEU	A	209	106.083	85.364	29.589	1.00 28.03	A
ATOM	1622	C	LEU	A	209	106.285	86.516	25.178	1.00 32.66	A
ATOM	1623	O	LEU	A	209	107.305	85.851	25.289	1.00 32.28	A
ATOM	1624	N	LYS	A	210	106.212	87.611	24.426	1.00 32.19	A
ATOM	1625	CA	LYS	A	210	107.337	88.134	23.658	1.00 34.20	A
ATOM	1626	CB	LYS	A	210	107.118	87.884	22.169	1.00 39.67	A
ATOM	1627	CG	LYS	A	210	106.844	86.472	21.772	1.00 49.14	A
ATOM	1628	CD	LYS	A	210	106.174	86.418	20.399	1.00 51.11	A
ATOM	1629	CE	LYS	A	210	106.928	85.462	19.474	1.00 58.79	A
ATOM	1630	NZ	LYS	A	210	106.158	85.113	18.241	1.00 57.80	A
ATOM	1631	C	LYS	A	210	107.421	89.644	23.793	1.00 35.59	A
ATOM	1632	O	LYS	A	210	106.520	90.290	24.326	1.00 39.70	A
ATOM	1633	N	GLY	A	211	108.488	90.201	23.230	1.00 37.65	A
ATOM	1634	CA	GLY	A	211	108.675	91.642	23.212	1.00 34.24	A
ATOM	1635	C	GLY	A	211	108.350	92.423	24.453	1.00 26.73	A
ATOM	1636	O	GLY	A	211	108.884	92.158	25.535	1.00 31.87	A
ATOM	1637	N	PRO	A	212	107.471	93.420	24.329	1.00 35.92	A
ATOM	1638	CD	PRO	A	212	106.750	93.851	23.117	1.00 36.64	A
ATOM	1639	CA	PRO	A	212	107.096	94.252	25.480	1.00 31.77	A
ATOM	1640	CB	PRO	A	212	106.113	95.266	24.881	1.00 34.18	A
ATOM	1641	CG	PRO	A	212	106.506	95.315	23.424	1.00 36.29	A
ATOM	1642	C	PRO	A	212	106.456	93.397	26.585	1.00 29.56	A
ATOM	1643	O	PRO	A	212	106.700	93.630	27.767	1.00 27.62	A
ATOM	1644	N	LEU	A	213	105.644	92.416	26.205	1.00 26.27	A
ATOM	1645	CA	LEU	A	213	105.036	91.569	27.232	1.00 30.09	A
ATOM	1646	CB	LEU	A	213	104.048	90.590	26.613	1.00 28.37	A
ATOM	1647	CG	LEU	A	213	102.726	91.280	26.223	1.00 31.49	A
ATOM	1648	CD1	LEU	A	213	102.970	92.306	25.101	1.00 29.76	A

ATOM	1649	CD2	LEU	A	213	101.738	90.239	25.745	1.00	29.45	A
ATOM	1650	C	LEU	A	213	106.112	90.830	28.032	1.00	22.05	A
ATOM	1651	O	LEU	A	213	106.139	90.886	29.250	1.00	25.06	A
ATOM	1652	N	LEU	A	214	107.023	90.176	27.331	1.00	29.37	A
ATOM	1653	CA	LEU	A	214	108.087	89.455	27.992	1.00	31.80	A
ATOM	1654	CB	LEU	A	214	109.030	88.849	26.952	1.00	27.44	A
ATOM	1655	CG	LEU	A	214	110.272	88.115	27.476	1.00	31.65	A
ATOM	1656	CD1	LEU	A	214	109.889	86.976	28.445	1.00	25.93	A
ATOM	1657	CD2	LEU	A	214	111.030	87.536	26.246	1.00	25.20	A
ATOM	1658	C	LEU	A	214	108.836	90.401	28.889	1.00	28.32	A
ATOM	1659	O	LEU	A	214	109.110	90.091	30.049	1.00	27.69	A
ATOM	1660	N	ASN	A	215	109.176	91.576	28.365	1.00	33.16	A
ATOM	1661	CA	ASN	A	215	109.912	92.553	29.175	1.00	30.08	A
ATOM	1662	CB	ASN	A	215	110.205	93.829	28.383	1.00	37.16	A
ATOM	1663	CG	ASN	A	215	110.980	94.815	29.205	1.00	39.99	A
ATOM	1664	OD1	ASN	A	215	112.161	94.586	29.516	1.00	38.55	A
ATOM	1665	ND2	ASN	A	215	110.311	95.895	29.629	1.00	39.72	A
ATOM	1666	C	ASN	A	215	109.189	92.951	30.453	1.00	26.60	A
ATOM	1667	O	ASN	A	215	109.789	93.055	31.522	1.00	27.99	A
ATOM	1668	N	LYS	A	216	107.891	93.204	30.346	1.00	29.96	A
ATOM	1669	CA	LYS	A	216	107.116	93.562	31.536	1.00	28.98	A
ATOM	1670	CB	LYS	A	216	105.669	93.842	31.124	1.00	27.44	A
ATOM	1671	CG	LYS	A	216	104.773	94.180	32.297	1.00	25.28	A
ATOM	1672	CD	LYS	A	216	103.384	94.434	31.799	1.00	29.65	A
ATOM	1673	CE	LYS	A	216	102.375	94.667	32.940	1.00	31.45	A
ATOM	1674	NZ	LYS	A	216	102.739	95.753	33.908	1.00	33.04	A
ATOM	1675	C	LYS	A	216	107.177	92.385	32.529	1.00	31.98	A
ATOM	1676	O	LYS	A	216	107.459	92.549	33.758	1.00	23.57	A
ATOM	1677	N	PHE	A	217	106.934	91.182	32.000	1.00	29.01	A
ATOM	1678	CA	PHE	A	217	106.984	90.002	32.862	1.00	23.20	A
ATOM	1679	CB	PHE	A	217	106.849	88.715	32.053	1.00	24.49	A
ATOM	1680	CG	PHE	A	217	107.137	87.453	32.855	1.00	30.86	A
ATOM	1681	CD1	PHE	A	217	106.184	86.923	33.729	1.00	25.74	A
ATOM	1682	CD2	PHE	A	217	108.350	86.762	32.682	1.00	33.51	A
ATOM	1683	CE1	PHE	A	217	106.418	85.718	34.410	1.00	27.69	A
ATOM	1684	CE2	PHE	A	217	108.598	85.553	33.359	1.00	30.90	A
ATOM	1685	CZ	PHE	A	217	107.620	85.029	34.228	1.00	26.68	A
ATOM	1686	C	PHE	A	217	108.277	89.949	33.655	1.00	25.85	A
ATOM	1687	O	PHE	A	217	108.255	89.888	34.892	1.00	26.90	A
ATOM	1688	N	LEU	A	218	109.417	90.010	32.967	1.00	29.26	A
ATOM	1689	CA	LEU	A	218	110.700	89.915	33.668	1.00	27.29	A
ATOM	1690	CB	LEU	A	218	111.853	89.742	32.671	1.00	29.60	A
ATOM	1691	CG	LEU	A	218	111.709	88.572	31.682	1.00	32.78	A
ATOM	1692	CD1	LEU	A	218	112.729	88.696	30.537	1.00	27.26	A
ATOM	1693	CD2	LEU	A	218	111.905	87.240	32.455	1.00	24.94	A
ATOM	1694	C	LEU	A	218	111.016	91.071	34.609	1.00	30.13	A
ATOM	1695	O	LEU	A	218	111.452	90.857	35.751	1.00	21.21	A
ATOM	1696	N	THR	A	219	110.798	92.295	34.141	1.00	31.78	A
ATOM	1697	CA	THR	A	219	111.097	93.480	34.958	1.00	35.74	A
ATOM	1698	CB	THR	A	219	112.082	94.772	34.097	1.00	33.10	A
ATOM	1699	OG1	THR	A	219	109.778	94.981	33.536	1.00	31.70	A
ATOM	1700	CG2	THR	A	219	112.106	94.645	32.947	1.00	34.85	A
ATOM	1701	C	THR	A	219	110.138	93.626	36.142	1.00	30.35	A
ATOM	1702	O	THR	A	219	110.431	94.334	37.101	1.00	30.89	A
ATOM	1703	N	THR	A	220	109.007	92.931	36.094	1.00	31.42	A

ATOM	1704	CA	THR	A	220	108.081	93.014	37.216	1.00	29.70	A
ATOM	1705	CB	THR	A	220	106.715	92.404	36.867	1.00	33.79	A
ATOM	1706	OG1	THR	A	220	106.091	93.206	35.862	1.00	29.37	A
ATOM	1707	CG2	THR	A	220	106.794	92.390	38.097	1.00	36.20	A
ATOM	1708	C	THR	A	220	108.666	92.314	38.437	1.00	30.26	A
ATOM	1709	O	THR	A	220	108.320	92.622	39.579	1.00	32.43	A
ATOM	1710	N	ALA	A	221	109.590	91.388	38.223	1.00	30.76	A
ATOM	1711	CA	ALA	A	221	110.140	90.711	39.383	1.00	33.31	A
ATOM	1712	CB	ALA	A	221	111.030	89.552	38.950	1.00	29.98	A
ATOM	1713	C	ALA	A	221	110.903	91.626	40.341	1.00	33.78	A
ATOM	1714	O	ALA	A	221	111.664	92.480	39.932	1.00	37.00	A
ATOM	1715	N	LYS	A	222	110.682	91.436	41.633	1.00	35.09	A
ATOM	1716	CA	LYS	A	222	111.385	92.202	42.645	1.00	35.18	A
ATOM	1717	CB	LYS	A	222	110.598	92.185	43.955	1.00	43.27	A
ATOM	1718	CG	LYS	A	222	111.085	93.202	44.970	1.00	51.49	A
ATOM	1719	CD	LYS	A	222	111.204	93.213	46.227	1.00	60.05	A
ATOM	1720	CE	LYS	A	222	110.402	94.508	47.040	1.00	63.10	A
ATOM	1721	NZ	LYS	A	222	111.855	94.791	47.290	1.00	63.82	A
ATOM	1722	C	LYS	A	222	113.740	91.534	42.864	1.00	39.12	A
ATOM	1723	O	LYS	A	222	113.811	90.313	43.020	1.00	31.62	A
ATOM	1724	N	ASP	A	223	114.809	92.332	42.906	1.00	35.35	A
ATOM	1725	CA	ASP	A	223	115.168	91.818	43.097	1.00	33.61	A
ATOM	1726	CB	ASP	A	223	115.383	91.275	44.518	1.00	42.55	A
ATOM	1727	CG	ASP	A	223	115.290	92.349	45.583	1.00	50.58	A
ATOM	1728	OD1	ASP	A	223	114.908	92.022	46.733	1.00	53.29	A
ATOM	1729	OD2	ASP	A	223	115.609	93.518	45.282	1.00	58.47	A
ATOM	1730	C	ASP	A	223	116.448	90.696	42.115	1.00	31.36	A
ATOM	1731	O	ASP	A	223	116.247	89.804	42.408	1.00	33.77	A
ATOM	1732	N	LYS	A	224	114.786	90.737	40.962	1.00	30.77	A
ATOM	1733	CA	LYS	A	224	114.964	89.706	39.940	1.00	35.01	A
ATOM	1734	CB	LYS	A	224	116.370	89.807	39.382	1.00	36.58	A
ATOM	1735	CG	LYS	A	224	116.693	91.208	38.878	1.00	47.96	A
ATOM	1736	CD	LYS	A	224	118.037	91.262	38.207	1.00	52.39	A
ATOM	1737	CE	LYS	A	224	118.284	92.622	37.573	1.00	56.76	A
ATOM	1738	NZ	LYS	A	224	117.429	92.538	36.606	1.00	59.77	A
ATOM	1739	C	LYS	A	224	114.720	88.268	40.446	1.00	35.05	A
ATOM	1740	O	LYS	A	224	115.159	87.296	39.832	1.00	31.24	A
ATOM	1741	N	ASN	A	225	114.026	88.117	41.566	1.00	27.53	A
ATOM	1742	CA	ASN	A	225	113.811	86.756	42.053	1.00	33.64	A
ATOM	1743	CB	ASN	A	225	114.834	86.408	43.156	1.00	24.93	A
ATOM	1744	CG	ASN	A	225	114.614	87.203	44.456	1.00	32.88	A
ATOM	1745	OD1	ASN	A	225	115.462	87.178	45.355	1.00	27.17	A
ATOM	1746	ND2	ASN	A	225	113.477	87.896	44.563	1.00	23.33	A
ATOM	1747	C	ASN	A	225	112.391	86.412	42.506	1.00	32.97	A
ATOM	1748	O	ASN	A	225	112.114	85.247	42.781	1.00	29.39	A
ATOM	1749	N	ARG	A	226	111.481	87.385	42.587	1.00	27.45	A
ATOM	1750	CA	ARG	A	226	110.126	87.028	43.007	1.00	24.16	A
ATOM	1751	CB	ARG	A	226	110.055	86.996	44.528	1.00	29.81	A
ATOM	1752	CG	ARG	A	226	110.358	88.346	45.221	1.00	29.04	A
ATOM	1753	CD	ARG	A	226	110.419	88.133	46.717	1.00	29.72	A
ATOM	1754	NE	ARG	A	226	110.694	89.338	47.493	1.00	36.06	A
ATOM	1755	CZ	ARG	A	226	111.862	89.992	47.530	1.00	40.98	A
ATOM	1756	NH1	ARG	A	226	112.909	89.572	46.818	1.00	42.69	A
ATOM	1757	NH2	ARG	A	226	111.994	91.066	48.310	1.00	37.88	A
ATOM	1758	C	ARG	A	226	109.069	87.973	42.477	1.00	31.57	A

ATOM	1759	O	ARG	A	226	109.330	89.143	42.211	1.00	25.27	A
ATOM	1760	N	TRP	A	227	107.867	87.456	42.299	1.00	28.37	A
ATOM	1761	CA	TRP	A	227	106.761	88.275	41.851	1.00	23.41	A
ATOM	1762	CB	TRP	A	227	105.973	87.536	40.760	1.00	20.74	A
ATOM	1763	CG	TRP	A	227	106.620	87.650	39.384	1.00	26.80	A
ATOM	1764	CD2	TRP	A	227	107.850	87.041	38.950	1.00	20.68	A
ATOM	1765	CE2	TRP	A	227	108.105	87.500	37.630	1.00	22.35	A
ATOM	1766	CE3	TRP	A	227	108.763	86.157	39.549	1.00	22.82	A
ATOM	1767	CD1	TRP	A	227	106.189	88.430	38.330	1.00	21.29	A
ATOM	1768	NE1	TRP	A	227	107.079	88.344	37.281	1.00	28.98	A
ATOM	1769	CZ2	TRP	A	227	109.225	87.105	36.897	1.00	24.84	A
ATOM	1770	CZ3	TRP	A	227	109.886	85.757	38.821	1.00	22.71	A
ATOM	1771	CH2	TRP	A	227	110.105	86.232	37.505	1.00	26.46	A
ATOM	1772	C	TRP	A	227	105.918	88.521	43.097	1.00	31.42	A
ATOM	1773	O	TRP	A	227	105.162	87.658	43.531	1.00	30.37	A
ATOM	1774	N	GLU	A	228	106.081	89.674	43.723	1.00	30.19	A
ATOM	1775	CA	GLU	A	228	105.278	89.914	44.897	1.00	40.90	A
ATOM	1776	CB	GLU	A	228	106.105	89.747	46.169	1.00	43.17	A
ATOM	1777	CG	GLU	A	228	107.143	90.767	46.430	1.00	49.83	A
ATOM	1778	CD	GLU	A	228	107.521	90.796	47.904	1.00	51.45	A
ATOM	1779	OE1	GLU	A	228	107.955	89.753	48.428	1.00	41.85	A
ATOM	1780	OE2	GLU	A	228	107.375	91.865	48.534	1.00	56.43	A
ATOM	1781	C	GLU	A	228	104.555	91.248	44.907	1.00	43.90	A
ATOM	1782	O	GLU	A	228	105.015	92.225	44.320	1.00	38.10	A
ATOM	1783	N	ASP	A	229	103.398	91.261	45.559	1.00	45.53	A
ATOM	1784	CA	ASP	A	229	102.606	92.462	45.661	1.00	49.47	A
ATOM	1785	CB	ASP	A	229	101.178	92.149	45.244	1.00	48.06	A
ATOM	1786	CG	ASP	A	229	101.057	91.972	43.727	1.00	50.49	A
ATOM	1787	OD1	ASP	A	229	101.471	92.917	43.003	1.00	49.52	A
ATOM	1788	OD2	ASP	A	229	100.573	90.910	43.263	1.00	34.83	A
ATOM	1789	C	ASP	A	229	102.716	92.944	47.097	1.00	56.94	A
ATOM	1790	O	ASP	A	229	102.511	94.165	48.033	1.00	47.42	A
ATOM	1791	N	PRO	A	230	103.104	94.229	47.290	1.00	64.41	A
ATOM	1792	CD	PRO	A	230	103.414	95.217	46.238	1.00	66.97	A
ATOM	1793	CA	PRO	A	230	103.241	94.830	48.625	1.00	64.83	A
ATOM	1794	CB	PRO	A	230	103.783	96.239	48.322	1.00	68.61	A
ATOM	1795	CG	PRO	A	230	103.206	96.530	46.968	1.00	71.34	A
ATOM	1796	C	PRO	A	230	101.958	94.835	49.400	1.00	61.61	A
ATOM	1797	O	PRO	A	230	100.886	94.963	48.819	1.00	59.14	A
ATOM	1798	N	GLY	A	231	102.066	94.671	50.713	1.00	64.01	A
ATOM	1799	CA	GLY	A	231	100.884	94.647	51.552	1.00	69.86	A
ATOM	1800	C	GLY	A	231	100.147	93.305	51.447	1.00	70.74	A
ATOM	1801	O	GLY	A	231	99.407	93.085	50.526	1.00	71.02	A
ATOM	1802	N	LYS	A	232	100.487	92.408	52.388	1.00	74.07	A
ATOM	1803	CA	LYS	A	232	99.884	91.088	52.345	1.00	77.87	A
ATOM	1804	CB	LYS	A	232	99.374	91.170	52.297	1.00	80.70	A
ATOM	1805	CG	LYS	A	232	97.722	91.539	53.624	1.00	83.42	A
ATOM	1806	CD	LYS	A	232	97.830	90.372	54.609	1.00	85.26	A
ATOM	1807	CE	LYS	A	232	97.028	90.622	55.884	1.00	85.21	A
ATOM	1808	NZ	LYS	A	232	97.013	89.416	56.769	1.00	86.74	A
ATOM	1809	C	LYS	A	232	100.443	90.345	51.087	1.00	77.00	A
ATOM	1810	O	LYS	A	232	99.701	89.982	50.156	1.00	76.48	A
ATOM	1811	N	GLN	A	233	101.762	90.168	51.071	1.00	70.42	A
ATOM	1812	CA	GLN	A	233	102.447	89.508	49.971	1.00	64.94	A
ATOM	1813	CB	GLN	A	233	103.805	89.999	49.916	1.00	65.15	A

ATOM	1814	CG	GLN	A	233	104.660	89.787	51.211	1.00	68.22	A
ATOM	1815	CD	GLN	A	233	105.334	91.059	51.716	1.00	73.51	A
ATOM	1816	OE1	GLN	A	233	106.256	91.581	51.087	1.00	79.17	A
ATOM	1817	NE2	GLN	A	233	104.869	91.567	52.359	1.00	73.37	A
ATOM	1818	C	GLN	A	233	102.416	88.003	50.192	1.00	62.45	A
ATOM	1819	O	GLN	A	233	103.423	87.332	50.007	1.00	59.36	A
ATOM	1820	N	LEU	A	234	101.267	87.473	50.604	1.00	59.16	A
ATOM	1821	CA	LEU	A	234	101.163	86.040	50.844	1.00	57.14	A
ATOM	1822	CB	LEU	A	234	100.011	85.733	51.808	1.00	58.67	A
ATOM	1823	CG	LEU	A	234	98.593	86.146	51.406	1.00	59.33	A
ATOM	1824	CD1	LEU	A	234	97.566	85.419	52.300	1.00	55.69	A
ATOM	1825	CD2	LEU	A	234	98.455	87.680	51.521	1.00	56.83	A
ATOM	1826	C	LEU	A	234	101.004	85.222	49.548	1.00	56.11	A
ATOM	1827	O	LEU	A	234	101.067	83.977	49.572	1.00	58.17	A
ATOM	1828	N	TYR	A	235	100.835	85.906	48.415	1.00	43.77	A
ATOM	1829	CA	TYR	A	235	100.694	85.205	47.142	1.00	33.72	A
ATOM	1830	CB	TYR	A	235	99.701	85.954	46.262	1.00	29.90	A
ATOM	1831	CG	TYR	A	235	98.416	86.253	46.982	1.00	31.05	A
ATOM	1832	CD1	TYR	A	235	97.805	87.505	46.872	1.00	32.37	A
ATOM	1833	CE1	TYR	A	235	96.614	87.785	47.530	1.00	27.48	A
ATOM	1834	CD2	TYR	A	235	97.799	85.273	47.779	1.00	29.78	A
ATOM	1835	CE2	TYR	A	235	96.615	85.533	48.437	1.00	27.57	A
ATOM	1836	CZ	TYR	A	235	96.026	86.789	48.303	1.00	33.50	A
ATOM	1837	OH	TYR	A	235	94.822	87.009	48.889	1.00	30.21	A
ATOM	1838	C	TYR	A	235	102.015	85.112	46.401	1.00	31.37	A
ATOM	1839	O	TYR	A	235	102.027	84.671	45.262	1.00	28.36	A
ATOM	1840	N	ASN	A	236	103.130	85.519	47.023	1.00	24.27	A
ATOM	1841	CA	ASN	A	236	104.399	85.505	46.292	1.00	20.44	A
ATOM	1842	CB	ASN	A	236	105.472	86.335	47.017	1.00	25.88	A
ATOM	1843	CG	ASN	A	236	105.651	85.944	48.484	1.00	30.25	A
ATOM	1844	OD1	ASN	A	236	104.890	85.148	49.032	1.00	39.82	A
ATOM	1845	ND2	ASN	A	236	106.644	86.543	49.133	1.00	28.85	A
ATOM	1846	C	ASN	A	236	104.955	84.137	45.960	1.00	20.82	A
ATOM	1847	O	ASN	A	236	105.588	83.968	44.919	1.00	20.31	A
ATOM	1848	N	VAL	A	237	104.761	83.155	46.831	1.00	20.09	A
ATOM	1849	CA	VAL	A	237	105.272	81.827	46.501	1.00	21.36	A
ATOM	1850	CB	VAL	A	237	105.154	80.861	47.704	1.00	18.71	A
ATOM	1851	CG1	VAL	A	237	105.601	79.471	47.312	1.00	14.08	A
ATOM	1852	CG2	VAL	A	237	106.052	81.376	48.846	1.00	27.50	A
ATOM	1853	C	VAL	A	237	104.481	81.299	45.301	1.00	18.56	A
ATOM	1854	O	VAL	A	237	105.063	80.794	44.343	1.00	18.22	A
ATOM	1855	N	GLU	A	238	103.162	81.479	45.323	1.00	17.79	A
ATOM	1856	CA	GLU	A	238	102.315	80.996	44.239	1.00	16.12	A
ATOM	1857	CB	GLU	A	238	100.824	81.147	44.601	1.00	17.19	A
ATOM	1858	CG	GLU	A	238	99.867	80.782	43.468	1.00	14.34	A
ATOM	1859	CD	GLU	A	238	98.471	81.420	43.650	1.00	11.06	A
ATOM	1860	OE1	GLU	A	238	98.241	82.107	44.686	1.00	19.48	A
ATOM	1861	OE2	GLU	A	238	97.621	81.200	42.783	1.00	16.80	A
ATOM	1862	C	GLU	A	238	102.628	81.744	42.958	1.00	20.05	A
ATOM	1863	O	GLU	A	238	102.815	81.130	41.897	1.00	18.11	A
ATOM	1864	N	ALA	A	239	102.684	83.071	43.036	1.00	18.43	A
ATOM	1865	CA	ALA	A	239	102.975	83.867	41.855	1.00	17.27	A
ATOM	1866	CB	ALA	A	239	102.988	85.340	42.221	1.00	17.99	A
ATOM	1867	C	ALA	A	239	104.334	83.488	41.251	1.00	16.91	A
ATOM	1868	O	ALA	A	239	104.510	83.248	40.038	1.00	18.31	A

ATOM	1869	N	THR	A	240	105.312	83.398	42.136	1.00	12.73	A
ATOM	1870	CA	THR	A	240	106.678	83.101	41.673	1.00	16.78	A
ATOM	1871	CB	THR	A	240	107.675	83.337	42.835	1.00	20.26	A
ATOM	1872	OG1	THR	A	240	107.499	84.683	43.322	1.00	20.23	A
ATOM	1873	CG2	THR	A	240	109.110	83.187	42.382	1.00	15.53	A
ATOM	1874	C	THR	A	240	106.790	81.686	41.087	1.00	23.59	A
ATOM	1875	O	THR	A	240	107.639	81.437	40.215	1.00	20.02	A
ATOM	1876	N	SER	A	241	105.941	80.760	41.552	1.00	15.58	A
ATOM	1877	CA	SER	A	241	105.991	79.381	41.022	1.00	17.43	A
ATOM	1878	CB	SER	A	241	105.162	78.441	41.906	1.00	11.67	A
ATOM	1879	OG	SER	A	241	105.715	78.363	43.233	1.00	15.93	A
ATOM	1880	C	SER	A	241	105.438	79.442	39.595	1.00	17.10	A
ATOM	1881	O	SER	A	241	105.980	78.810	38.675	1.00	18.31	A
ATOM	1882	N	TYR	A	242	104.365	80.217	39.383	1.00	18.46	A
ATOM	1883	CA	TYR	A	242	103.846	80.367	38.013	1.00	18.91	A
ATOM	1884	CB	TYR	A	242	102.622	81.307	37.942	1.00	15.98	A
ATOM	1885	CG	TYR	A	242	101.263	80.652	38.190	1.00	20.69	A
ATOM	1886	CD1	TYR	A	242	100.766	79.658	37.338	1.00	13.29	A
ATOM	1887	CE1	TYR	A	242	99.504	79.043	37.567	1.00	18.13	A
ATOM	1888	CD2	TYR	A	242	100.486	81.030	39.086	1.00	16.91	A
ATOM	1889	CE2	TYR	A	242	99.246	80.434	39.537	1.00	11.03	A
ATOM	1890	CZ	TYR	A	242	98.759	79.444	38.669	1.00	19.17	A
ATOM	1891	OH	TYR	A	242	97.505	78.916	38.898	1.00	17.62	A
ATOM	1892	C	TYR	A	242	104.949	81.000	37.157	1.00	23.33	A
ATOM	1893	O	TYR	A	242	105.190	80.603	35.997	1.00	22.29	A
ATOM	1894	N	ALA	A	243	105.613	82.004	37.717	1.00	18.34	A
ATOM	1895	CA	ALA	A	243	106.634	82.697	36.929	1.00	18.89	A
ATOM	1896	CB	ALA	A	243	107.164	83.901	37.694	1.00	19.57	A
ATOM	1897	C	ALA	A	243	107.772	81.717	36.609	1.00	21.61	A
ATOM	1898	O	ALA	A	243	108.290	81.731	35.494	1.00	21.45	A
ATOM	1899	N	LEU	A	244	108.145	80.861	37.565	1.00	16.89	A
ATOM	1900	CA	LEU	A	244	109.239	79.899	37.309	1.00	20.89	A
ATOM	1901	CB	LEU	A	244	109.588	79.103	38.587	1.00	16.59	A
ATOM	1902	CG	LEU	A	244	110.578	77.933	38.379	1.00	21.10	A
ATOM	1903	CD1	LEU	A	244	111.844	78.449	37.632	1.00	20.05	A
ATOM	1904	CD2	LEU	A	244	110.974	77.326	39.777	1.00	12.73	A
ATOM	1905	C	LEU	A	244	108.813	78.947	36.182	1.00	18.67	A
ATOM	1906	O	LEU	A	244	109.610	78.556	35.296	1.00	19.02	A
ATOM	1907	N	LEU	A	245	107.542	78.574	36.181	1.00	17.68	A
ATOM	1908	CA	LEU	A	245	107.074	77.709	35.107	1.00	15.21	A
ATOM	1909	CB	LEU	A	245	105.628	77.214	35.404	1.00	20.70	A
ATOM	1910	CG	LEU	A	245	105.557	76.123	36.506	1.00	21.76	A
ATOM	1911	CD1	LEU	A	245	104.108	75.956	36.996	1.00	26.34	A
ATOM	1912	CD2	LEU	A	245	106.100	74.778	35.969	1.00	16.28	A
ATOM	1913	C	LEU	A	245	107.147	78.449	33.[illegible]	1.00	19.30	A
ATOM	1914	O	LEU	A	245	107.449	77.831	32.717	1.00	20.79	A
ATOM	1915	N	ALA	A	246	106.874	79.759	33.704	1.00	18.12	A
ATOM	1916	CA	ALA	A	246	106.959	80.501	32.461	1.00	18.77	A
ATOM	1917	CB	ALA	A	246	106.367	81.944	32.633	1.00	16.45	A
ATOM	1918	C	ALA	A	246	108.431	80.558	32.009	1.00	14.13	A
ATOM	1919	O	ALA	A	246	108.738	80.352	30.823	1.00	19.75	A
ATOM	1920	N	LEU	A	247	109.337	80.835	32.944	1.00	15.08	A
ATOM	1921	CA	LEU	A	247	110.769	80.899	32.620	1.00	18.36	A
ATOM	1922	CB	LEU	A	247	111.567	81.267	33.866	1.00	19.66	A
ATOM	1923	CG	LEU	A	247	111.365	82.715	34.363	1.00	20.28	A

ATOM	1924	CD1	LEU	A	247	111.874	82.820	35.813	1.00	17.02	A
ATOM	1925	CD2	LEU	A	247	112.098	83.725	33.441	1.00	21.44	A
ATOM	1926	C	LEU	A	247	111.263	79.557	32.058	1.00	23.09	A
ATOM	1927	O	LEU	A	247	112.038	79.526	31.092	1.00	25.65	A
ATOM	1928	N	LEU	A	248	110.796	78.447	32.624	1.00	22.19	A
ATOM	1929	CA	LEU	A	248	111.239	77.124	32.123	1.00	23.05	A
ATOM	1930	CB	LEU	A	248	110.815	75.977	33.081	1.00	24.02	A
ATOM	1931	CG	LEU	A	248	111.577	75.998	34.437	1.00	25.05	A
ATOM	1932	CD1	LEU	A	248	110.943	75.071	35.436	1.00	24.06	A
ATOM	1933	CD2	LEU	A	248	113.066	75.617	34.216	1.00	15.01	A
ATOM	1934	C	LEU	A	248	110.657	76.914	30.745	1.00	23.21	A
ATOM	1935	O	LEU	A	248	111.313	76.391	29.847	1.00	25.42	A
ATOM	1936	N	GLN	A	249	109.416	77.324	30.572	1.00	22.82	A
ATOM	1937	CA	GLN	A	249	108.757	77.197	29.281	1.00	22.86	A
ATOM	1938	CB	GLN	A	249	107.314	77.694	29.377	1.00	27.58	A
ATOM	1939	CG	GLN	A	249	106.526	77.545	28.085	1.00	34.66	A
ATOM	1940	CD	GLN	A	249	106.170	76.085	27.789	1.00	39.67	A
ATOM	1941	OE1	GLN	A	249	105.459	75.434	28.554	1.00	44.37	A
ATOM	1942	NE2	GLN	A	249	106.672	75.575	26.687	1.00	37.71	A
ATOM	1943	C	GLN	A	249	109.513	78.042	28.226	1.00	27.62	A
ATOM	1944	O	GLN	A	249	109.623	77.655	27.079	1.00	24.60	A
ATOM	1945	N	LEU	A	250	110.009	79.207	28.618	1.00	32.08	A
ATOM	1946	CA	LEU	A	250	110.740	80.080	27.700	1.00	30.59	A
ATOM	1947	CB	LEU	A	250	110.736	81.501	28.247	1.00	28.66	A
ATOM	1948	CG	LEU	A	250	109.401	82.220	28.410	1.00	30.11	A
ATOM	1949	CD1	LEU	A	250	109.530	83.326	29.426	1.00	29.85	A
ATOM	1950	CD2	LEU	A	250	108.960	82.728	27.062	1.00	28.49	A
ATOM	1951	C	LEU	A	250	112.207	79.647	27.551	1.00	36.31	A
ATOM	1952	O	LEU	A	250	112.938	80.189	26.708	1.00	31.07	A
ATOM	1953	N	LYS	A	251	112.627	78.682	28.373	1.00	30.98	A
ATOM	1954	CA	LYS	A	251	114.016	78.226	28.410	1.00	31.57	A
ATOM	1955	CB	LYS	A	251	114.420	77.554	27.098	1.00	32.85	A
ATOM	1956	CG	LYS	A	251	113.715	76.232	26.890	1.00	42.53	A
ATOM	1957	CD	LYS	A	251	114.060	75.631	25.555	1.00	46.71	A
ATOM	1958	CE	LYS	A	251	113.233	74.376	25.314	1.00	54.63	A
ATOM	1959	NZ	LYS	A	251	113.214	73.987	23.864	1.00	58.25	A
ATOM	1960	C	LYS	A	251	114.943	79.412	28.712	1.00	31.12	A
ATOM	1961	O	LYS	A	251	116.102	79.442	28.301	1.00	32.07	A
ATOM	1962	N	ASP	A	252	114.438	80.376	29.479	1.00	29.36	A
ATOM	1963	CA	ASP	A	252	115.239	81.521	29.830	1.00	28.62	A
ATOM	1964	CB	ASP	A	252	114.346	82.738	30.091	1.00	33.61	A
ATOM	1965	CG	ASP	A	252	115.150	84.017	30.237	1.00	37.36	A
ATOM	1966	OD1	ASP	A	252	116.328	83.990	29.839	1.00	49.12	A
ATOM	1967	OD2	ASP	A	252	114.624	85.048	30.725	1.00	34.68	A
ATOM	1968	C	ASP	A	252	116.097	81.183	31.046	1.00	31.99	A
ATOM	1969	O	ASP	A	252	115.933	81.742	32.139	1.00	30.76	A
ATOM	1970	N	PHE	A	253	117.069	80.301	30.819	1.00	31.40	A
ATOM	1971	CA	PHE	A	253	117.935	79.818	31.873	1.00	27.03	A
ATOM	1972	CB	PHE	A	253	118.786	78.674	31.338	1.00	33.08	A
ATOM	1973	CG	PHE	A	253	117.995	77.601	30.649	1.00	33.23	A
ATOM	1974	CD1	PHE	A	253	116.815	77.109	31.205	1.00	35.86	A
ATOM	1975	CD2	PHE	A	253	118.460	77.032	29.463	1.00	34.30	A
ATOM	1976	CE1	PHE	A	253	116.115	76.061	30.593	1.00	35.38	A
ATOM	1977	CE2	PHE	A	253	117.762	75.987	28.853	1.00	30.02	A
ATOM	1978	CZ	PHE	A	253	116.593	75.504	29.421	1.00	32.95	A

ATOM	1979	C	PHE	A	253	118.823	80.800	32.619	1.00	36.01	A
ATOM	1980	O	PHE	A	253	119.249	80.512	33.746	1.00	32.40	A
ATOM	1981	N	ASP	A	254	119.124	81.951	32.028	1.00	33.64	A
ATOM	1982	CA	ASP	A	254	119.986	82.905	32.728	1.00	37.81	A
ATOM	1983	CB	ASP	A	254	120.588	83.884	31.729	1.00	49.35	A
ATOM	1984	CG	ASP	A	254	119.539	84.520	30.871	1.00	65.34	A
ATOM	1985	OD1	ASP	A	254	118.936	83.793	30.046	1.00	75.38	A
ATOM	1986	OD2	ASP	A	254	119.293	85.740	31.023	1.00	75.70	A
ATOM	1987	C	ASP	A	254	119.210	83.669	33.802	1.00	31.65	A
ATOM	1988	O	ASP	A	254	119.791	84.196	34.752	1.00	30.63	A
ATOM	1989	N	PHE	A	255	117.892	83.728	33.652	1.00	28.90	A
ATOM	1990	CA	PHE	A	255	117.058	84.442	34.616	1.00	29.25	A
ATOM	1991	CB	PHE	A	255	115.881	85.100	33.892	1.00	28.92	A
ATOM	1992	CG	PHE	A	255	115.234	86.213	34.671	1.00	38.13	A
ATOM	1993	CD1	PHE	A	255	114.281	85.947	35.643	1.00	31.13	A
ATOM	1994	CD2	PHE	A	255	115.596	87.546	34.432	1.00	39.51	A
ATOM	1995	CE1	PHE	A	255	113.695	86.988	36.366	1.00	38.06	A
ATOM	1996	CE2	PHE	A	255	115.017	88.589	35.150	1.00	35.88	A
ATOM	1997	CZ	PHE	A	255	114.063	88.313	36.120	1.00	39.10	A
ATOM	1998	C	PHE	A	255	116.523	83.530	35.721	1.00	28.15	A
ATOM	1999	O	PHE	A	255	116.078	83.996	36.767	1.00	27.42	A
ATOM	2000	N	VAL	A	256	116.562	82.228	35.482	1.00	24.41	A
ATOM	2001	CA	VAL	A	256	116.040	81.257	36.453	1.00	21.90	A
ATOM	2002	CB	VAL	A	256	116.017	79.838	35.789	1.00	26.19	A
ATOM	2003	CG1	VAL	A	256	115.894	78.725	36.829	1.00	17.67	A
ATOM	2004	CG2	VAL	A	256	114.827	79.770	34.812	1.00	22.75	A
ATOM	2005	C	VAL	A	256	116.666	81.130	37.848	1.00	22.10	A
ATOM	2006	O	VAL	A	256	115.946	81.095	38.871	1.00	28.02	A
ATOM	2007	N	PRO	A	257	118.007	81.124	37.931	1.00	21.20	A
ATOM	2008	CD	PRO	A	257	118.995	81.442	36.886	1.00	24.71	A
ATOM	2009	CA	PRO	A	257	118.667	80.963	39.234	1.00	24.35	A
ATOM	2010	CB	PRO	A	257	120.169	81.097	38.899	1.00	27.97	A
ATOM	2011	CG	PRO	A	257	120.234	80.711	37.411	1.00	23.95	A
ATOM	2012	C	PRO	A	257	118.258	81.802	40.403	1.00	24.79	A
ATOM	2013	O	PRO	A	257	117.988	81.266	41.468	1.00	27.34	A
ATOM	2014	N	PRO	A	258	118.189	83.134	40.250	1.00	25.57	A
ATOM	2015	CD	PRO	A	258	118.491	84.076	39.165	1.00	26.97	A
ATOM	2016	CA	PRO	A	258	117.785	83.828	41.487	1.00	25.28	A
ATOM	2017	CB	PRO	A	258	117.840	85.322	41.103	1.00	29.92	A
ATOM	2018	CG	PRO	A	258	118.862	85.363	39.944	1.00	31.32	A
ATOM	2019	C	PRO	A	258	116.373	83.414	41.927	1.00	25.27	A
ATOM	2020	O	PRO	A	258	116.032	83.438	43.117	1.00	21.56	A
ATOM	2021	N	VAL	A	259	115.552	83.013	40.963	1.00	21.83	A
ATOM	2022	CA	VAL	A	259	114.175	82.658	41.291	1.00	22.97	A
ATOM	2023	CB	VAL	A	259	113.339	82.571	39.988	1.00	21.99	A
ATOM	2024	CG1	VAL	A	259	111.917	82.096	40.294	1.00	17.20	A
ATOM	2025	CG2	VAL	A	259	113.271	83.961	39.346	1.00	24.31	A
ATOM	2026	C	VAL	A	259	114.069	81.353	42.085	1.00	19.11	A
ATOM	2027	O	VAL	A	259	113.366	81.256	43.091	1.00	32.76	A
ATOM	2028	N	VAL	A	260	114.783	80.357	41.620	1.00	26.91	A
ATOM	2029	CA	VAL	A	260	114.760	79.071	42.275	1.00	24.36	A
ATOM	2030	CB	VAL	A	260	115.564	78.094	41.451	1.00	23.58	A
ATOM	2031	CG1	VAL	A	260	115.723	76.787	42.189	1.00	24.55	A
ATOM	2032	CG2	VAL	A	260	114.865	77.887	40.155	1.00	21.01	A
ATOM	2033	C	VAL	A	260	115.340	79.231	43.657	1.00	24.01	A

ATOM	2034	O	VAL	A	260	114.815	78.721	44.651	1.00	20.85	A
ATOM	2035	N	ARG	A	261	116.436	79.972	43.724	1.00	24.50	A
ATOM	2036	CA	ARG	A	261	117.084	80.219	45.002	1.00	19.29	A
ATOM	2037	CB	ARG	A	261	118.320	81.101	44.757	1.00	26.10	A
ATOM	2038	CG	ARG	A	261	119.216	81.291	45.956	1.00	42.29	A
ATOM	2039	CD	ARG	A	261	120.449	82.133	45.594	1.00	48.37	A
ATOM	2040	NE	ARG	A	261	121.239	81.474	44.553	1.00	53.77	A
ATOM	2041	CZ	ARG	A	261	121.406	81.910	43.301	1.00	58.06	A
ATOM	2042	NH1	ARG	A	261	120.845	83.045	42.877	1.00	55.53	A
ATOM	2043	NH2	ARG	A	261	122.128	81.180	42.454	1.00	54.87	A
ATOM	2044	C	ARG	A	261	116.114	80.883	45.999	1.00	26.55	A
ATOM	2045	O	ARG	A	261	116.056	80.507	47.169	1.00	25.37	A
ATOM	2046	N	TRP	A	262	115.353	81.885	45.556	1.00	21.10	A
ATOM	2047	CA	TRP	A	262	114.423	82.526	46.469	1.00	21.13	A
ATOM	2048	CB	TRP	A	262	113.759	83.756	45.804	1.00	27.41	A
ATOM	2049	CG	TRP	A	262	112.747	84.440	46.710	1.00	26.23	A
ATOM	2050	CD2	TRP	A	262	111.344	84.176	46.770	1.00	24.38	A
ATOM	2051	CE2	TRP	A	262	110.809	84.949	47.839	1.00	22.85	A
ATOM	2052	CE3	TRP	A	262	110.479	83.359	46.027	1.00	29.17	A
ATOM	2053	CD1	TRP	A	262	113.008	85.351	47.715	1.00	27.15	A
ATOM	2054	NE1	TRP	A	262	111.844	85.659	48.397	1.00	25.55	A
ATOM	2055	CZ2	TRP	A	262	109.458	84.922	48.177	1.00	22.55	A
ATOM	2056	CZ3	TRP	A	262	109.134	83.332	46.359	1.00	22.37	A
ATOM	2057	CH2	TRP	A	262	108.636	84.106	47.427	1.00	27.32	A
ATOM	2058	C	TRP	A	262	113.345	81.504	46.891	1.00	21.59	A
ATOM	2059	O	TRP	A	262	113.003	81.383	48.077	1.00	21.98	A
ATOM	2060	N	LEU	A	263	112.806	80.767	45.927	1.00	24.29	A
ATOM	2061	CA	LEU	A	263	111.760	79.775	46.248	1.00	24.58	A
ATOM	2062	CB	LEU	A	263	111.270	79.050	44.985	1.00	23.15	A
ATOM	2063	CG	LEU	A	263	110.294	79.804	44.055	1.00	26.66	A
ATOM	2064	CD1	LEU	A	263	110.179	79.064	42.702	1.00	25.63	A
ATOM	2065	CD2	LEU	A	263	108.902	79.890	44.736	1.00	19.50	A
ATOM	2066	C	LEU	A	263	112.280	78.754	47.252	1.00	25.46	A
ATOM	2067	O	LEU	A	263	111.589	78.396	48.213	1.00	21.54	A
ATOM	2068	N	ASN	A	264	113.521	78.334	47.052	1.00	27.69	A
ATOM	2069	CA	ASN	A	264	114.138	77.339	47.923	1.00	26.89	A
ATOM	2070	CB	ASN	A	264	115.429	76.833	47.317	1.00	30.52	A
ATOM	2071	CG	ASN	A	264	115.869	75.523	47.906	1.00	37.07	A
ATOM	2072	OD1	ASN	A	264	117.047	75.355	48.181	1.00	41.85	A
ATOM	2073	ND2	ASN	A	264	114.936	74.576	48.093	1.00	34.54	A
ATOM	2074	C	ASN	A	264	114.426	77.843	49.308	1.00	31.72	A
ATOM	2075	O	ASN	A	264	114.734	77.040	50.186	1.00	29.93	A
ATOM	2076	N	GLU	A	265	114.368	79.161	49.518	1.00	23.33	A
ATOM	2077	CA	GLU	A	265	114.583	79.677	50.868	1.00	27.89	A
ATOM	2078	CB	GLU	A	265	115.256	81.057	50.817	1.00	36.54	A
ATOM	2079	CG	GLU	A	265	116.666	81.031	50.220	1.00	45.81	A
ATOM	2080	CD	GLU	A	265	117.203	82.426	49.890	1.00	52.24	A
ATOM	2081	OE1	GLU	A	265	116.112	83.284	49.448	1.00	55.22	A
ATOM	2082	OE2	GLU	A	265	118.421	82.659	50.052	1.00	59.70	A
ATOM	2083	C	GLU	A	265	113.240	79.794	51.617	1.00	31.76	A
ATOM	2084	O	GLU	A	265	113.210	80.100	52.800	1.00	31.51	A
ATOM	2085	N	GLN	A	266	112.131	79.578	50.917	1.00	25.12	A
ATOM	2086	CA	GLN	A	266	110.823	79.682	51.534	1.00	25.11	A
ATOM	2087	CB	GLN	A	266	109.769	80.120	50.492	1.00	22.70	A
ATOM	2088	CG	GLN	A	266	110.160	81.344	49.619	1.00	27.84	A

ATOM	2089	CD	GLN	A	266	110.749	82.499	50.434	1.00	30.91	A
ATOM	2090	OE1	GLN	A	266	110.138	82.961	51.386	1.00	29.87	A
ATOM	2091	NE2	GLN	A	266	111.949	82.952	50.065	1.00	23.36	A
ATOM	2092	C	GLN	A	266	110.402	78.343	52.166	1.00	29.30	A
ATOM	2093	O	GLN	A	266	110.826	77.247	51.730	1.00	24.87	A
ATOM	2094	N	ARG	A	267	109.585	78.444	53.212	1.00	15.92	A
ATOM	2095	CA	ARG	A	267	109.051	77.274	53.898	1.00	25.35	A
ATOM	2096	CB	ARG	A	267	108.588	77.693	55.292	1.00	33.71	A
ATOM	2097	CG	ARG	A	267	107.994	76.574	56.134	1.00	51.92	A
ATOM	2098	CD	ARG	A	267	107.907	76.988	57.616	1.00	62.06	A
ATOM	2099	NE	ARG	A	267	106.792	76.336	58.312	1.00	68.36	A
ATOM	2100	CZ	ARG	A	267	105.511	76.589	58.055	1.00	69.62	A
ATOM	2101	NH1	ARG	A	267	105.199	77.484	57.118	1.00	71.28	A
ATOM	2102	NH2	ARG	A	267	104.546	75.951	58.721	1.00	63.27	A
ATOM	2103	C	ARG	A	267	107.868	76.833	53.031	1.00	24.21	A
ATOM	2104	O	ARG	A	267	106.740	76.727	53.500	1.00	21.31	A
ATOM	2105	N	TYR	A	268	108.146	76.503	51.772	1.00	20.68	A
ATOM	2106	CA	TYR	A	268	107.077	76.220	50.844	1.00	19.61	A
ATOM	2107	CB	TYR	A	268	107.623	76.325	49.416	1.00	19.65	A
ATOM	2108	CG	TYR	A	268	108.603	75.213	49.054	1.00	20.48	A
ATOM	2109	CD1	TYR	A	268	108.141	73.919	48.758	1.00	14.04	A
ATOM	2110	CE1	TYR	A	268	109.038	72.914	48.336	1.00	17.07	A
ATOM	2111	CD2	TYR	A	268	109.988	75.469	48.950	1.00	18.73	A
ATOM	2112	CE2	TYR	A	268	110.896	74.462	48.562	1.00	10.52	A
ATOM	2113	CZ	TYR	A	268	110.400	73.191	48.251	1.00	18.28	A
ATOM	2114	OH	TYR	A	268	111.270	72.207	47.849	1.00	20.44	A
ATOM	2115	C	TYR	A	268	106.320	74.921	51.058	1.00	25.67	A
ATOM	2116	O	TYR	A	268	105.280	74.726	50.457	1.00	20.64	A
ATOM	2117	N	TYR	A	269	106.837	74.047	51.923	1.00	22.96	A
ATOM	2118	CA	TYR	A	269	106.192	72.764	52.224	1.00	22.56	A
ATOM	2119	CB	TYR	A	269	107.284	71.749	52.550	1.00	19.40	A
ATOM	2120	CG	TYR	A	269	108.279	72.324	53.538	1.00	25.20	A
ATOM	2121	CD1	TYR	A	269	108.002	72.326	54.913	1.00	21.63	A
ATOM	2122	CE1	TYR	A	269	108.856	72.951	55.823	1.00	19.42	A
ATOM	2123	CD2	TYR	A	269	109.452	72.970	53.098	1.00	23.97	A
ATOM	2124	CE2	TYR	A	269	110.310	73.620	54.010	1.00	18.32	A
ATOM	2125	CZ	TYR	A	269	110.002	73.600	55.359	1.00	24.42	A
ATOM	2126	OH	TYR	A	269	110.809	74.232	56.269	1.00	30.40	A
ATOM	2127	C	TYR	A	269	105.286	72.941	53.459	1.00	19.68	A
ATOM	2128	O	TYR	A	269	104.703	71.986	53.943	1.00	21.53	A
ATOM	2129	N	GLY	A	270	105.176	74.170	53.948	1.00	21.67	A
ATOM	2130	CA	GLY	A	270	104.406	74.456	55.146	1.00	17.59	A
ATOM	2131	C	GLY	A	270	102.977	73.953	55.184	1.00	25.69	A
ATOM	2132	O	GLY	A	270	102.532	73.482	56.232	1.00	24.34	A
ATOM	2133	N	GLY	A	271	102.266	73.984	54.057	1.00	19.73	A
ATOM	2134	CA	GLY	A	271	100.868	73.577	54.104	1.00	21.41	A
ATOM	2135	C	GLY	A	271	100.160	74.574	55.033	1.00	26.85	A
ATOM	2136	O	GLY	A	271	100.583	75.740	55.198	1.00	40.08	A
ATOM	2137	N	GLY	A	272	99.091	74.158	55.662	1.00	23.80	A
ATOM	2138	CA	GLY	A	272	98.437	75.085	56.568	1.00	26.88	A
ATOM	2139	C	GLY	A	272	97.305	75.856	55.915	1.00	23.11	A
ATOM	2140	O	GLY	A	272	97.123	75.787	54.712	1.00	21.50	A
ATOM	2141	N	TYR	A	273	96.567	76.618	56.710	1.00	17.15	A
ATOM	2142	CA	TYR	A	273	95.425	77.353	56.196	1.00	19.83	A
ATOM	2143	CB	TYR	A	273	94.836	78.198	57.313	1.00	21.62	A

ATOM	2144	CG	TYR	A	273	93.616	78.988	56.897	1.00	23.29	A
ATOM	2145	CD1	TYR	A	273	92.321	78.473	57.084	1.00	20.57	A
ATOM	2146	CE1	TYR	A	273	91.184	79.246	56.758	1.00	23.40	A
ATOM	2147	CD2	TYR	A	273	93.759	80.281	56.359	1.00	23.31	A
ATOM	2148	CE2	TYR	A	273	92.646	81.060	56.027	1.00	22.47	A
ATOM	2149	CZ	TYR	A	273	91.371	80.532	56.235	1.00	20.88	A
ATOM	2150	OH	TYR	A	273	90.314	81.304	55.896	1.00	20.65	A
ATOM	2151	C	TYR	A	273	95.747	78.224	54.976	1.00	23.07	A
ATOM	2152	O	TYR	A	273	96.764	78.920	54.931	1.00	14.66	A
ATOM	2153	N	GLY	A	274	94.891	78.150	53.966	1.00	23.18	A
ATOM	2154	CA	GLY	A	274	95.092	78.955	52.768	1.00	16.12	A
ATOM	2155	C	GLY	A	274	96.280	78.623	51.891	1.00	25.88	A
ATOM	2156	O	GLY	A	274	96.629	79.431	51.012	1.00	20.78	A
ATOM	2157	N	SER	A	275	96.907	77.458	52.080	1.00	14.86	A
ATOM	2158	CA	SER	A	275	98.089	77.131	51.270	1.00	20.55	A
ATOM	2159	CB	SER	A	275	99.074	76.297	52.077	1.00	16.52	A
ATOM	2160	OG	SER	A	275	98.428	75.061	52.389	1.00	21.60	A
ATOM	2161	C	SER	A	275	97.806	76.335	50.005	1.00	20.94	A
ATOM	2162	O	SER	A	275	98.746	75.961	49.318	1.00	17.86	A
ATOM	2163	N	THR	A	276	96.544	76.072	49.683	1.00	18.41	A
ATOM	2164	CA	THR	A	276	96.269	75.232	48.516	1.00	19.71	A
ATOM	2165	CB	THR	A	276	94.730	75.059	48.238	1.00	22.45	A
ATOM	2166	OG1	THR	A	276	94.192	76.301	47.838	1.00	51.89	A
ATOM	2167	CG2	THR	A	276	93.993	74.729	49.503	1.00	5.81	A
ATOM	2168	C	THR	A	276	96.967	75.607	47.228	1.00	21.51	A
ATOM	2169	O	THR	A	276	97.666	74.764	46.650	1.00	19.94	A
ATOM	2170	N	GLN	A	277	96.823	76.850	46.754	1.00	13.97	A
ATOM	2171	CA	GLN	A	277	97.463	77.189	45.485	1.00	15.27	A
ATOM	2172	CB	GLN	A	277	96.942	78.540	44.964	1.00	15.99	A
ATOM	2173	CG	GLN	A	277	95.421	78.529	44.563	1.00	8.40	A
ATOM	2174	CD	GLN	A	277	95.100	77.321	43.742	1.00	20.22	A
ATOM	2175	OE1	GLN	A	277	95.685	77.090	42.673	1.00	16.53	A
ATOM	2176	NE2	GLN	A	277	94.190	76.505	44.258	1.00	18.51	A
ATOM	2177	C	GLN	A	277	99.007	77.229	45.567	1.00	13.58	A
ATOM	2178	O	GLN	A	277	99.689	76.791	44.620	1.00	15.16	A
ATOM	2179	N	ALA	A	278	99.534	77.754	46.667	1.00	17.70	A
ATOM	2180	CA	ALA	A	278	100.996	77.842	46.833	1.00	17.58	A
ATOM	2181	CB	ALA	A	278	101.367	78.532	48.200	1.00	12.12	A
ATOM	2182	C	ALA	A	278	101.539	76.426	46.798	1.00	20.92	A
ATOM	2183	O	ALA	A	278	102.581	76.154	46.176	1.00	19.56	A
ATOM	2184	N	THR	A	279	100.821	75.534	47.477	1.00	18.75	A
ATOM	2185	CA	THR	A	279	101.254	74.136	47.553	1.00	15.04	A
ATOM	2186	CB	THR	A	279	100.380	73.341	48.554	1.00	23.60	A
ATOM	2187	OG1	THR	A	279	100.574	73.865	49.873	1.00	16.00	A
ATOM	2188	CG2	THR	A	279	100.755	71.832	48.531	1.00	18.05	A
ATOM	2189	C	THR	A	279	101.224	73.469	46.195	1.00	20.78	A
ATOM	2190	O	THR	A	279	102.224	72.834	45.758	1.00	14.58	A
ATOM	2191	N	PHE	A	280	100.080	73.544	45.514	1.00	14.85	A
ATOM	2192	CA	PHE	A	280	99.989	72.925	44.212	1.00	15.92	A
ATOM	2193	CB	PHE	A	280	98.601	73.198	43.604	1.00	15.13	A
ATOM	2194	CG	PHE	A	280	98.354	72.463	42.313	1.00	19.65	A
ATOM	2195	CD1	PHE	A	280	97.543	71.341	42.284	1.00	19.12	A
ATOM	2196	CD2	PHE	A	280	98.873	72.932	41.120	1.00	17.17	A
ATOM	2197	CE1	PHE	A	280	97.261	70.703	41.074	1.00	21.16	A
ATOM	2198	CE2	PHE	A	280	98.593	72.308	39.910	1.00	22.94	A

ATOM	2199	CZ	PHE	A	280	97.784	71.202	39.884	1.00	22.80	A
ATOM	2200	C	PHE	A	280	101.031	73.493	43.273	1.00	22.45	A
ATOM	2201	O	PHE	A	280	101.706	72.768	42.534	1.00	17.39	A
ATOM	2202	N	MET	A	281	101.157	74.808	43.284	1.00	15.49	A
ATOM	2203	CA	MET	A	281	102.061	75.445	42.339	1.00	19.30	A
ATOM	2204	CB	MET	A	281	101.681	76.939	42.169	1.00	16.61	A
ATOM	2205	CG	MET	A	281	100.322	77.212	41.527	1.00	18.78	A
ATOM	2206	SD	MET	A	281	100.020	76.356	39.946	1.00	24.71	A
ATOM	2207	CE	MET	A	281	101.567	76.615	39.056	1.00	22.61	A
ATOM	2208	C	MET	A	281	103.576	75.321	42.559	1.00	12.99	A
ATOM	2209	O	MET	A	281	104.316	75.044	41.593	1.00	20.36	A
ATOM	2210	N	VAL	A	282	104.036	75.481	43.800	1.00	20.60	A
ATOM	2211	CA	VAL	A	282	105.475	75.395	44.084	1.00	17.17	A
ATOM	2212	CB	VAL	A	282	105.795	75.806	45.562	1.00	16.00	A
ATOM	2213	CG1	VAL	A	282	105.366	74.677	46.522	1.00	16.44	A
ATOM	2214	CG2	VAL	A	282	107.331	76.108	45.740	1.00	20.08	A
ATOM	2215	C	VAL	A	282	105.974	73.961	43.790	1.00	16.69	A
ATOM	2216	O	VAL	A	282	107.058	73.777	43.230	1.00	16.91	A
ATOM	2217	N	PHE	A	283	105.184	72.943	44.134	1.00	13.38	A
ATOM	2218	CA	PHE	A	283	105.623	71.562	43.832	1.00	20.74	A
ATOM	2219	CB	PHE	A	283	104.821	70.541	44.684	1.00	13.63	A
ATOM	2220	CG	PHE	A	283	105.280	70.495	46.117	1.00	21.60	A
ATOM	2221	CD1	PHE	A	283	104.633	71.260	47.107	1.00	18.08	A
ATOM	2222	CD2	PHE	A	283	106.402	69.732	46.477	1.00	17.18	A
ATOM	2223	CE1	PHE	A	283	105.100	71.264	48.441	1.00	21.58	A
ATOM	2224	CE2	PHE	A	283	106.873	69.736	47.809	1.00	19.10	A
ATOM	2225	CZ	PHE	A	283	106.220	70.502	48.790	1.00	15.19	A
ATOM	2226	C	PHE	A	283	105.559	71.274	42.329	1.00	17.88	A
ATOM	2227	O	PHE	A	283	106.418	70.582	41.780	1.00	17.08	A
ATOM	2228	N	GLN	A	284	104.572	71.859	41.642	1.00	17.15	A
ATOM	2229	CA	GLN	A	284	104.505	71.696	40.195	1.00	15.23	A
ATOM	2230	CB	GLN	A	284	103.258	72.375	39.570	1.00	19.08	A
ATOM	2231	CG	GLN	A	284	103.135	72.123	38.053	1.00	13.61	A
ATOM	2232	CD	GLN	A	284	101.834	72.642	37.446	1.00	27.56	A
ATOM	2233	OE1	GLN	A	284	101.215	73.561	37.957	1.00	19.72	A
ATOM	2234	NE2	GLN	A	284	101.419	72.040	36.358	1.00	28.76	A
ATOM	2235	C	GLN	A	284	105.733	72.350	39.583	1.00	23.26	A
ATOM	2236	O	GLN	A	284	106.403	71.749	38.721	1.00	19.38	A
ATOM	2237	N	ALA	A	285	106.032	73.586	40.020	1.00	20.27	A
ATOM	2238	CA	ALA	A	285	107.169	74.314	39.474	1.00	22.72	A
ATOM	2239	CB	ALA	A	285	107.131	75.841	39.900	1.00	13.58	A
ATOM	2240	C	ALA	A	285	108.525	73.704	39.796	1.00	19.56	A
ATOM	2241	O	ALA	A	285	109.342	73.571	38.891	1.00	18.63	A
ATOM	2242	N	LEU	A	286	108.775	73.348	41.060	1.00	17.53	A
ATOM	2243	CA	LEU	A	286	110.059	72.729	41.426	1.00	22.71	A
ATOM	2244	CB	LEU	A	286	110.038	72.682	42.957	1.00	20.14	A
ATOM	2245	CG	LEU	A	286	110.227	74.014	43.563	1.00	26.93	A
ATOM	2246	CD1	LEU	A	286	110.528	74.003	45.093	1.00	20.46	A
ATOM	2247	CD2	LEU	A	286	111.470	74.793	42.896	1.00	21.22	A
ATOM	2248	C	LEU	A	286	110.181	71.322	40.832	1.00	18.99	A
ATOM	2249	O	LEU	A	286	111.286	70.866	40.558	1.00	23.33	A
ATOM	2250	N	ALA	A	287	109.058	70.631	40.629	1.00	20.11	A
ATOM	2251	CA	ALA	A	287	109.135	69.321	39.980	1.00	18.27	A
ATOM	2252	CB	ALA	A	287	107.786	68.606	40.005	1.00	16.55	A
ATOM	2253	C	ALA	A	287	109.519	69.613	38.530	1.00	25.56	A

ATOM	2254	O	ALA	A	287	110.381	68.942	37.927	1.00	19.06	A
ATOM	2255	N	GLN	A	288	108.907	70.634	37.935	1.00	18.68	A
ATOM	2256	CA	GLN	A	288	109.249	70.877	36.536	1.00	16.52	A
ATOM	2257	CB	GLN	A	288	108.392	71.977	35.894	1.00	22.21	A
ATOM	2258	CG	GLN	A	288	108.681	72.106	34.390	1.00	20.99	A
ATOM	2259	CD	GLN	A	288	108.188	70.889	33.579	1.00	24.85	A
ATOM	2260	OE1	GLN	A	288	108.896	70.370	32.704	1.00	24.90	A
ATOM	2261	NE2	GLN	A	288	106.972	70.448	33.863	1.00	18.47	A
ATOM	2262	C	GLN	A	288	110.719	71.258	36.345	1.00	22.79	A
ATOM	2263	O	GLN	A	288	111.330	70.907	35.335	1.00	16.55	A
ATOM	2264	N	TYR	A	289	111.262	72.009	37.287	1.00	19.12	A
ATOM	2265	CA	TYR	A	289	112.654	72.405	37.203	1.00	18.73	A
ATOM	2266	CB	TYR	A	289	113.021	73.260	38.403	1.00	18.19	A
ATOM	2267	CG	TYR	A	289	114.482	73.677	38.476	1.00	26.27	A
ATOM	2268	CD1	TYR	A	289	114.898	74.932	38.001	1.00	26.71	A
ATOM	2269	CE1	TYR	A	289	116.232	75.332	38.072	1.00	25.07	A
ATOM	2270	CD2	TYR	A	289	115.447	72.820	39.024	1.00	23.61	A
ATOM	2271	CE2	TYR	A	289	116.796	73.199	39.098	1.00	26.68	A
ATOM	2272	CZ	TYR	A	289	117.178	74.469	38.615	1.00	31.54	A
ATOM	2273	OH	TYR	A	289	118.491	74.859	38.678	1.00	22.55	A
ATOM	2274	C	TYR	A	289	113.541	71.142	37.207	1.00	25.66	A
ATOM	2275	O	TYR	A	289	114.502	71.042	36.424	1.00	21.35	A
ATOM	2276	N	GLN	A	290	113.224	70.195	38.095	1.00	23.15	A
ATOM	2277	CA	GLN	A	290	114.013	68.974	38.200	1.00	25.92	A
ATOM	2278	CB	GLN	A	290	113.751	68.295	39.535	1.00	16.82	A
ATOM	2279	CG	GLN	A	290	114.234	69.185	40.698	1.00	20.11	A
ATOM	2280	CD	GLN	A	290	113.869	68.620	42.062	1.00	28.81	A
ATOM	2281	OE1	GLN	A	290	114.594	67.805	42.611	1.00	23.19	A
ATOM	2282	NE2	GLN	A	290	112.740	69.050	42.603	1.00	19.24	A
ATOM	2283	C	GLN	A	290	113.792	68.037	37.053	1.00	24.56	A
ATOM	2284	O	GLN	A	290	114.690	67.272	36.654	1.00	31.99	A
ATOM	2285	N	LYS	A	291	112.604	68.100	36.485	1.00	28.20	A
ATOM	2286	CA	LYS	A	291	112.340	67.233	35.349	1.00	27.92	A
ATOM	2287	CB	LYS	A	291	110.879	67.253	34.960	1.00	25.58	A
ATOM	2288	CG	LYS	A	291	110.640	66.179	33.951	1.00	35.43	A
ATOM	2289	CD	LYS	A	291	109.644	66.601	32.962	1.00	47.83	A
ATOM	2290	CE	LYS	A	291	109.438	65.497	31.950	1.00	54.06	A
ATOM	2291	NZ	LYS	A	291	108.781	64.338	32.602	1.00	54.26	A
ATOM	2292	C	LYS	A	291	113.128	67.716	34.138	1.00	30.13	A
ATOM	2293	O	LYS	A	291	113.543	66.915	33.313	1.00	24.65	A
ATOM	2294	N	ASP	A	292	113.305	69.031	34.028	1.00	21.05	A
ATOM	2295	CA	ASP	A	292	114.016	69.633	32.891	1.00	25.19	A
ATOM	2296	CB	ASP	A	292	113.610	71.109	32.757	1.00	23.19	A
ATOM	2297	CG	ASP	A	292	112.222	71.299	32.158	1.00	33.23	A
ATOM	2298	OD1	ASP	A	292	111.626	70.308	31.703	1.00	27.34	A
ATOM	2299	OD2	ASP	A	292	111.737	72.452	32.131	1.00	27.83	A
ATOM	2300	C	ASP	A	292	115.556	69.584	33.008	1.00	23.90	A
ATOM	2301	O	ASP	A	292	116.275	69.573	32.017	1.00	22.32	A
ATOM	2302	N	ALA	A	293	116.034	69.604	34.236	1.00	20.48	A
ATOM	2303	CA	ALA	A	293	117.451	69.602	34.558	1.00	28.06	A
ATOM	2304	CB	ALA	A	293	117.602	69.472	36.065	1.00	20.35	A
ATOM	2305	C	ALA	A	293	118.355	68.564	33.838	1.00	29.15	A
ATOM	2306	O	ALA	A	293	119.480	68.885	33.427	1.00	30.95	A
ATOM	2307	N	PRO	A	294	117.913	67.302	33.732	1.00	29.07	A
ATOM	2308	CD	PRO	A	294	116.811	66.630	34.437	1.00	30.66	A

ATOM	2309	CA	PRO	A	294	118.777	66.331	33.051	1.00	28.43	A
ATOM	2310	CB	PRO	A	294	118.013	65.019	33.196	1.00	36.12	A
ATOM	2311	CG	PRO	A	294	117.307	65.185	34.516	1.00	34.80	A
ATOM	2312	C	PRO	A	294	119.062	66.686	31.593	1.00	34.08	A
ATOM	2313	O	PRO	A	294	120.059	66.245	31.042	1.00	37.55	A
ATOM	2314	N	SER	A	295	118.206	67.496	30.970	1.00	31.59	A
ATOM	2315	CA	SER	A	295	118.412	67.895	29.570	1.00	32.05	A
ATOM	2316	CB	SER	A	295	117.053	68.031	28.827	1.00	37.77	A
ATOM	2317	OG	SER	A	295	116.413	66.791	28.542	1.00	38.35	A
ATOM	2318	C	SER	A	295	119.141	69.246	29.412	1.00	33.12	A
ATOM	2319	O	SER	A	295	119.543	69.592	28.310	1.00	27.93	A
ATOM	2320	N	ASP	A	296	119.310	70.014	30.490	1.00	26.80	A
ATOM	2321	CA	ASP	A	296	119.913	71.328	30.352	1.00	30.74	A
ATOM	2322	CB	ASP	A	296	118.782	72.415	30.256	1.00	27.90	A
ATOM	2323	CG	ASP	A	296	117.839	72.252	28.986	1.00	41.52	A
ATOM	2324	OD1	ASP	A	296	118.246	72.564	27.834	1.00	38.56	A
ATOM	2325	OD2	ASP	A	296	116.655	71.816	29.121	1.00	44.60	A
ATOM	2326	C	ASP	A	296	120.862	71.604	31.525	1.00	31.76	A
ATOM	2327	O	ASP	A	296	120.426	71.809	32.661	1.00	31.22	A
ATOM	2328	N	HIS	A	297	122.161	71.613	31.240	1.00	27.39	A
ATOM	2329	CA	HIS	A	297	123.221	71.862	32.231	1.00	31.02	A
ATOM	2330	CB	HIS	A	297	124.562	72.043	31.514	1.00	39.25	A
ATOM	2331	CG	HIS	A	297	125.466	70.858	31.577	1.00	47.23	A
ATOM	2332	CD2	HIS	A	297	126.818	70.762	31.501	1.00	46.79	A
ATOM	2333	ND1	HIS	A	297	125.005	69.597	31.863	1.00	48.20	A
ATOM	2334	CE1	HIS	A	297	126.036	68.777	31.990	1.00	54.99	A
ATOM	2335	NE2	HIS	A	297	127.146	69.462	31.778	1.00	46.54	A
ATOM	2336	C	HIS	A	297	122.999	73.125	33.043	1.00	27.48	A
ATOM	2337	O	HIS	A	297	123.412	73.224	34.203	1.00	28.00	A
ATOM	2338	N	GLN	A	298	122.396	74.117	32.401	1.00	22.60	A
ATOM	2339	CA	GLN	A	298	122.174	75.396	33.046	1.00	25.08	A
ATOM	2340	CB	GLN	A	298	121.569	76.409	32.065	1.00	30.41	A
ATOM	2341	CG	GLN	A	298	120.332	76.669	30.783	1.00	34.42	A
ATOM	2342	CD	GLN	A	298	121.872	75.791	29.603	1.00	37.26	A
ATOM	2343	OE1	GLN	A	298	121.932	76.217	28.444	1.00	36.98	A
ATOM	2344	NE2	GLN	A	298	121.429	74.558	29.897	1.00	32.64	A
ATOM	2345	C	GLN	A	298	121.276	75.302	34.280	1.00	26.28	A
ATOM	2346	O	GLN	A	298	121.322	76.182	35.129	1.00	23.86	A
ATOM	2347	N	GLU	A	299	120.448	74.263	34.374	1.00	22.71	A
ATOM	2348	CA	GLU	A	299	119.556	74.107	35.525	1.00	29.56	A
ATOM	2349	CB	GLU	A	299	118.247	73.497	35.081	1.00	27.09	A
ATOM	2350	CG	GLU	A	299	117.445	74.443	34.288	1.00	42.75	A
ATOM	2351	CD	GLU	A	299	116.372	73.723	33.574	1.00	52.61	A
ATOM	2352	OE1	GLU	A	299	115.342	73.415	34.208	1.00	64.24	A
ATOM	2353	OE2	GLU	A	299	116.565	73.443	32.377	1.00	59.69	A
ATOM	2354	C	GLU	A	299	120.251	73.185	36.491	1.00	30.34	A
ATOM	2355	O	GLU	A	299	119.841	72.042	36.706	1.00	25.19	A
ATOM	2356	N	LEU	A	300	121.289	73.724	37.099	1.00	26.72	A
ATOM	2357	CA	LEU	A	300	122.164	72.950	37.960	1.00	26.15	A
ATOM	2358	CB	LEU	A	300	123.621	73.384	37.693	1.00	24.26	A
ATOM	2359	CG	LEU	A	300	124.040	74.875	37.817	1.00	23.41	A
ATOM	2360	CD1	LEU	A	300	122.894	75.782	38.110	1.00	13.62	A
ATOM	2361	CD2	LEU	A	300	125.064	75.023	38.845	1.00	23.86	A
ATOM	2362	C	LEU	A	300	121.930	73.005	39.439	1.00	31.66	A
ATOM	2363	O	LEU	A	300	122.685	72.360	40.165	1.00	24.27	A

ATOM	2364	N	ASN	A	301	120.399	73.717	39.895	1.00	20.86	A
ATOM	2365	CA	ASN	A	301	120.674	73.844	41.335	1.00	27.51	A
ATOM	2366	CB	ASN	A	301	119.685	74.974	41.629	1.00	27.49	A
ATOM	2367	CG	ASN	A	301	120.338	76.367	41.606	1.00	41.50	A
ATOM	2368	OD1	ASN	A	301	121.514	76.531	41.948	1.00	42.07	A
ATOM	2369	ND2	ASN	A	301	119.545	77.386	41.248	1.00	40.89	A
ATOM	2370	C	ASN	A	301	120.139	72.561	41.946	1.00	27.36	A
ATOM	2371	O	ASN	A	301	119.478	71.775	41.255	1.00	20.70	A
ATOM	2372	N	LEU	A	302	120.455	72.338	43.227	1.00	28.60	A
ATOM	2373	CA	LEU	A	302	119.962	71.168	43.945	1.00	24.52	A
ATOM	2374	CB	LEU	A	302	121.038	70.593	44.894	1.00	29.03	A
ATOM	2375	CG	LEU	A	302	120.446	69.605	45.935	1.00	27.91	A
ATOM	2376	CD1	LEU	A	302	119.494	68.711	45.254	1.00	18.13	A
ATOM	2377	CD2	LEU	A	302	121.464	68.809	46.627	1.00	28.47	A
ATOM	2378	C	LEU	A	302	118.742	71.586	44.767	1.00	21.88	A
ATOM	2379	O	LEU	A	302	118.898	72.203	45.817	1.00	20.14	A
ATOM	2380	N	ASP	A	303	117.540	71.265	44.306	1.00	18.15	A
ATOM	2381	CA	ASP	A	303	116.335	71.611	45.095	1.00	29.52	A
ATOM	2382	CB	ASP	A	303	115.472	72.630	44.334	1.00	25.17	A
ATOM	2383	CG	ASP	A	303	115.065	72.121	42.996	1.00	37.89	A
ATOM	2384	OD1	ASP	A	303	115.528	71.037	42.637	1.00	54.39	A
ATOM	2385	OD2	ASP	A	303	114.248	72.780	42.279	1.00	57.27	A
ATOM	2386	C	ASP	A	303	115.580	70.289	45.373	1.00	22.29	A
ATOM	2387	O	ASP	A	303	114.347	70.216	45.577	1.00	22.75	A
ATOM	2388	N	VAL	A	304	116.382	69.240	45.425	1.00	21.19	A
ATOM	2389	CA	VAL	A	304	115.905	67.870	45.624	1.00	25.10	A
ATOM	2390	CB	VAL	A	304	116.935	66.930	44.914	1.00	21.32	A
ATOM	2391	CG1	VAL	A	304	118.001	66.444	45.851	1.00	13.87	A
ATOM	2392	CG2	VAL	A	304	116.235	65.842	44.282	1.00	42.05	A
ATOM	2393	C	VAL	A	304	115.770	67.499	47.102	1.00	19.73	A
ATOM	2394	O	VAL	A	304	116.213	68.242	47.961	1.00	19.32	A
ATOM	2395	N	SER	A	305	115.136	66.360	47.402	1.00	21.55	A
ATOM	2396	CA	SER	A	305	114.969	65.904	48.794	1.00	24.92	A
ATOM	2397	CB	SER	A	305	114.202	64.572	48.838	1.00	31.82	A
ATOM	2398	OG	SER	A	305	112.797	64.716	48.530	1.00	45.40	A
ATOM	2399	C	SER	A	305	116.366	65.696	49.401	1.00	32.11	A
ATOM	2400	O	SER	A	305	117.187	64.961	48.836	1.00	19.54	A
ATOM	2401	N	LEU	A	306	116.649	66.330	50.535	1.00	25.35	A
ATOM	2402	CA	LEU	A	306	117.962	66.173	51.161	1.00	30.33	A
ATOM	2403	CB	LEU	A	306	118.422	67.488	51.831	1.00	35.23	A
ATOM	2404	CG	LEU	A	306	118.886	68.694	50.987	1.00	33.58	A
ATOM	2405	CD1	LEU	A	306	119.870	68.352	49.838	1.00	29.73	A
ATOM	2406	CD2	LEU	A	306	117.665	69.257	50.434	1.00	39.98	A
ATOM	2407	C	LEU	A	306	117.913	65.050	52.208	1.00	37.07	A
ATOM	2408	O	LEU	A	306	116.871	64.515	52.547	1.00	34.47	A
ATOM	2409	N	GLN	A	307	119.107	64.670	52.722	1.00	37.78	A
ATOM	2410	CA	GLN	A	307	119.102	63.615	53.734	1.00	47.24	A
ATOM	2411	CB	GLN	A	307	121.517	63.110	54.035	1.00	52.95	A
ATOM	2412	CG	GLN	A	307	120.931	61.932	53.174	1.00	64.46	A
ATOM	2413	CD	GLN	A	307	121.481	62.371	51.846	1.00	70.87	A
ATOM	2414	OE1	GLN	A	307	122.341	63.253	51.785	1.00	76.28	A
ATOM	2415	NE2	GLN	A	307	121.001	61.755	50.767	1.00	77.08	A
ATOM	2416	C	GLN	A	307	118.462	64.115	55.021	1.00	42.93	A
ATOM	2417	O	GLN	A	307	118.665	65.308	55.340	1.00	42.42	A
ATOM	2418	OXT	GLN	A	307	117.838	63.294	55.699	1.00	44.41	A

ATOM	2419	CB	ALA	B	1	64.181	107.666	4.123	1.00	39.20	B
ATOM	2420	C	ALA	B	1	62.836	105.816	3.113	1.00	41.03	B
ATOM	2421	O	ALA	B	1	61.659	105.713	3.477	1.00	42.08	B
ATOM	2422	N	ALA	B	1	62.413	108.231	2.458	1.00	40.18	B
ATOM	2423	CA	ALA	B	1	63.447	107.201	2.861	1.00	43.96	B
ATOM	2424	N	ILE	B	2	63.636	104.759	2.923	1.00	39.63	B
ATOM	2425	CA	ILE	B	2	63.175	103.383	3.141	1.00	37.01	B
ATOM	2426	CB	ILE	B	2	64.245	102.349	2.700	1.00	32.57	B
ATOM	2427	CG2	ILE	B	2	63.775	100.936	3.064	1.00	35.80	B
ATOM	2428	CG1	ILE	B	2	64.457	102.422	1.178	1.00	34.01	B
ATOM	2429	CD1	ILE	B	2	65.479	101.372	0.650	1.00	31.21	B
ATOM	2430	C	ILE	B	2	62.831	103.151	4.633	1.00	38.27	B
ATOM	2431	O	ILE	B	2	63.565	103.577	5.528	1.00	32.71	B
ATOM	2432	N	SER	B	3	61.714	102.486	4.897	1.00	30.65	B
ATOM	2433	CA	SER	B	3	61.316	102.226	6.272	1.00	26.19	B
ATOM	2434	CB	SER	B	3	60.245	103.236	6.689	1.00	31.79	B
ATOM	2435	OG	SER	B	3	59.060	103.029	5.926	1.00	27.35	B
ATOM	2436	C	SER	B	3	60.744	100.825	6.435	1.00	30.38	B
ATOM	2437	O	SER	B	3	60.495	100.132	5.446	1.00	28.89	B
ATOM	2438	N	CYS	B	4	60.559	100.410	7.690	1.00	27.89	B
ATOM	2439	CA	CYS	B	4	59.941	99.127	8.003	1.00	27.29	B
ATOM	2440	C	CYS	B	4	58.609	99.528	8.600	1.00	26.13	B
ATOM	2441	O	CYS	B	4	58.446	100.666	9.061	1.00	29.64	B
ATOM	2442	CB	CYS	B	4	60.731	98.328	9.056	1.00	27.46	B
ATOM	2443	SG	CYS	B	4	62.214	97.531	8.369	1.00	27.76	B
ATOM	2444	N	GLY	B	5	57.648	98.600	8.561	1.00	22.65	B
ATOM	2445	CA	GLY	B	5	56.366	98.916	9.155	1.00	23.57	B
ATOM	2446	C	GLY	B	5	56.452	98.570	10.643	1.00	24.00	B
ATOM	2447	O	GLY	B	5	57.504	98.199	11.181	1.00	23.18	B
ATOM	2448	N	SER	B	6	55.322	98.698	11.313	1.00	21.65	B
ATOM	2449	CA	SER	B	6	55.204	98.441	12.733	1.00	22.23	B
ATOM	2450	CB	SER	B	6	53.722	98.511	13.098	1.00	27.49	B
ATOM	2451	OG	SER	B	6	53.543	98.605	14.483	1.00	33.82	B
ATOM	2452	C	SER	B	6	55.785	97.062	13.091	1.00	26.45	B
ATOM	2453	O	SER	B	6	55.489	96.081	12.439	1.00	22.14	B
ATOM	2454	N	PRO	B	7	56.639	96.980	14.122	1.00	26.74	B
ATOM	2455	CD	PRO	B	7	57.230	98.026	14.973	1.00	25.89	B
ATOM	2456	CA	PRO	B	7	57.191	95.661	14.468	1.00	25.01	B
ATOM	2457	CB	PRO	B	7	58.175	95.984	15.592	1.00	22.52	B
ATOM	2458	CG	PRO	B	7	57.589	97.228	16.232	1.00	26.49	B
ATOM	2459	C	PRO	B	7	56.133	94.627	14.894	1.00	27.04	B
ATOM	2460	O	PRO	B	7	55.061	94.961	15.414	1.00	24.19	B
ATOM	2461	N	PRO	B	8	56.439	93.345	14.700	1.00	24.37	B
ATOM	2462	CD	PRO	B	8	57.540	92.754	13.936	1.00	26.75	B
ATOM	2463	CA	PRO	B	8	55.431	92.366	15.099	1.00	25.28	B
ATOM	2464	CB	PRO	B	8	55.974	91.048	14.538	1.00	31.15	B
ATOM	2465	CG	PRO	B	8	57.401	91.314	14.245	1.00	33.33	B
ATOM	2466	C	PRO	B	8	55.228	92.382	16.613	1.00	30.70	B
ATOM	2467	O	PRO	B	8	56.180	92.527	17.364	1.00	31.22	B
ATOM	2468	N	PRO	B	9	53.971	92.214	17.074	1.00	30.39	B
ATOM	2469	CD	PRO	B	9	52.724	92.280	16.275	1.00	37.82	B
ATOM	2470	CA	PRO	B	9	53.686	92.322	18.518	1.00	32.22	B
ATOM	2471	CB	PRO	B	9	52.155	92.415	18.589	1.00	31.66	B
ATOM	2472	CG	PRO	B	9	51.705	91.731	17.265	1.00	31.37	B
ATOM	2473	C	PRO	B	9	54.190	91.062	19.209	1.00	26.54	B

ATOM	2474	O	PRO	B	9	54.542	90.072	18.563	1.00	23.13	B
ATOM	2475	N	ILE	B	10	54.214	91.111	20.526	1.00	25.96	B
ATOM	2476	CA	ILE	B	10	54.651	89.969	21.302	1.00	34.36	B
ATOM	2477	CB	ILE	B	10	56.150	90.068	21.770	1.00	24.92	B
ATOM	2478	CG2	ILE	B	10	56.398	91.363	22.561	1.00	24.04	B
ATOM	2479	CG1	ILE	B	10	56.491	88.795	22.581	1.00	30.43	B
ATOM	2480	CD1	ILE	B	10	57.991	88.536	22.813	1.00	24.83	B
ATOM	2481	C	ILE	B	10	53.753	89.810	22.511	1.00	33.31	B
ATOM	2482	O	ILE	B	10	53.743	90.647	23.412	1.00	32.83	B
ATOM	2483	N	LEU	B	11	52.992	88.724	22.525	1.00	30.71	B
ATOM	2484	CA	LEU	B	11	52.108	88.483	23.659	1.00	34.63	B
ATOM	2485	CB	LEU	B	11	51.217	87.277	23.365	1.00	36.50	B
ATOM	2486	CG	LEU	B	11	50.279	87.435	22.161	1.00	41.37	B
ATOM	2487	CD1	LEU	B	11	49.708	86.073	21.769	1.00	42.99	B
ATOM	2488	CD2	LEU	B	11	49.142	88.425	22.495	1.00	39.65	B
ATOM	2489	C	LEU	B	11	52.912	88.247	24.946	1.00	33.29	B
ATOM	2490	O	LEU	B	11	53.905	87.517	24.948	1.00	28.06	B
ATOM	2491	N	ASN	B	12	52.463	88.872	26.032	1.00	31.32	B
ATOM	2492	CA	ASN	B	12	53.086	88.753	27.328	1.00	30.29	B
ATOM	2493	CB	ASN	B	12	53.025	87.303	27.802	1.00	32.27	B
ATOM	2494	CG	ASN	B	12	51.612	86.875	28.083	1.00	38.86	B
ATOM	2495	OD1	ASN	B	12	50.917	87.526	28.864	1.00	38.55	B
ATOM	2496	ND2	ASN	B	12	51.161	85.805	27.431	1.00	34.66	B
ATOM	2497	C	ASN	B	12	54.510	89.250	27.371	1.00	32.36	B
ATOM	2498	O	ASN	B	12	55.277	88.858	28.239	1.00	32.55	B
ATOM	2499	N	GLY	B	13	54.849	90.130	26.439	1.00	28.46	B
ATOM	2500	CA	GLY	B	13	56.187	90.671	26.400	1.00	28.72	B
ATOM	2501	C	GLY	B	13	56.147	92.166	26.169	1.00	29.82	B
ATOM	2502	O	GLY	B	13	55.075	92.780	26.153	1.00	34.03	B
ATOM	2503	N	ARG	B	14	57.324	92.742	25.983	1.00	28.15	B
ATOM	2504	CA	ARG	B	14	57.486	94.166	25.739	1.00	31.15	B
ATOM	2505	CB	ARG	B	14	58.198	94.882	26.897	1.00	34.62	B
ATOM	2506	CG	ARG	B	14	57.388	95.196	28.126	1.00	41.44	B
ATOM	2507	CD	ARG	B	14	58.240	95.962	29.112	1.00	42.08	B
ATOM	2508	NE	ARG	B	14	57.526	96.080	30.373	1.00	49.55	B
ATOM	2509	CZ	ARG	B	14	58.023	96.595	31.487	1.00	48.40	B
ATOM	2510	NH1	ARG	B	14	59.261	97.065	31.509	1.00	40.73	B
ATOM	2511	NH2	ARG	B	14	57.276	96.602	32.595	1.00	56.30	B
ATOM	2512	C	ARG	B	14	58.409	94.342	24.557	1.00	23.56	B
ATOM	2513	O	ARG	B	14	59.232	93.480	24.280	1.00	23.51	B
ATOM	2514	N	ILE	B	15	58.319	95.516	23.955	1.00	27.48	B
ATOM	2515	CA	ILE	B	15	59.171	95.893	22.841	1.00	26.75	B
ATOM	2516	CB	ILE	B	15	58.345	96.176	21.580	1.00	26.32	B
ATOM	2517	CG2	ILE	B	15	59.250	96.815	20.497	1.00	29.30	B
ATOM	2518	CG1	ILE	B	15	57.656	94.902	21.120	1.00	30.62	B
ATOM	2519	CD1	ILE	B	15	56.760	95.100	19.889	1.00	35.23	B
ATOM	2520	C	ILE	B	15	59.767	97.212	23.279	1.00	26.59	B
ATOM	2521	O	ILE	B	15	59.050	98.050	23.818	1.00	30.94	B
ATOM	2522	N	SER	B	16	61.055	97.409	23.036	1.00	25.15	B
ATOM	2523	CA	SER	B	16	61.709	98.654	23.393	1.00	32.61	B
ATOM	2524	CB	SER	B	16	63.187	98.567	23.057	1.00	29.32	B
ATOM	2525	OG	SER	B	16	63.359	98.151	21.717	1.00	35.31	B
ATOM	2526	C	SER	B	16	61.082	99.839	22.639	1.00	41.27	B
ATOM	2527	O	SER	B	16	60.466	99.674	21.576	1.00	36.78	B
ATOM	2528	N	TYR	B	17	61.260	101.035	23.193	1.00	42.89	B

ATOM	2529	CA	TYR	B	17	60.719	102.267	22.624	1.00	46.29	B
ATOM	2530	CB	TYR	B	17	60.932	103.436	23.623	1.00	44.99	B
ATOM	2531	CG	TYR	B	17	60.026	103.380	24.865	1.00	47.02	B
ATOM	2532	CD1	TYR	B	17	60.510	103.694	26.151	1.00	49.03	B
ATOM	2533	CE1	TYR	B	17	59.664	103.655	27.283	1.00	48.52	B
ATOM	2534	CD2	TYR	B	17	58.686	103.025	24.748	1.00	51.67	B
ATOM	2535	CE2	TYR	B	17	57.833	102.974	25.861	1.00	53.32	B
ATOM	2536	CZ	TYR	B	17	58.319	103.292	27.122	1.00	56.82	B
ATOM	2537	OH	TYR	B	17	57.430	103.259	28.190	1.00	55.53	B
ATOM	2538	C	TYR	B	17	61.397	102.551	21.285	1.00	46.15	B
ATOM	2539	O	TYR	B	17	62.600	102.375	21.146	1.00	50.00	B
ATOM	2540	N	TYR	B	18	60.623	102.952	20.281	1.00	46.05	B
ATOM	2541	CA	TYR	B	18	61.204	103.270	18.975	1.00	44.93	B
ATOM	2542	CB	TYR	B	18	61.076	102.076	18.010	1.00	37.78	B
ATOM	2543	CG	TYR	B	18	59.645	101.669	17.711	1.00	37.10	B
ATOM	2544	CD1	TYR	B	18	58.890	102.343	16.750	1.00	31.24	B
ATOM	2545	CE1	TYR	B	18	57.573	101.980	16.501	1.00	34.43	B
ATOM	2546	CD2	TYR	B	18	59.040	100.622	18.415	1.00	34.57	B
ATOM	2547	CE2	TYR	B	18	57.730	100.255	18.184	1.00	36.06	B
ATOM	2548	CZ	TYR	B	18	57.000	100.939	17.218	1.00	35.02	B
ATOM	2549	OH	TYR	B	18	55.706	100.565	16.967	1.00	33.22	B
ATOM	2550	C	TYR	B	18	60.524	104.514	18.375	1.00	40.62	B
ATOM	2551	O	TYR	B	18	59.356	104.784	18.632	1.00	40.57	B
ATOM	2552	N	SER	B	19	61.280	105.260	17.586	1.00	42.39	B
ATOM	2553	CA	SER	B	19	60.786	106.464	16.931	1.00	48.17	B
ATOM	2554	CB	SER	B	19	61.922	107.472	16.789	1.00	49.59	B
ATOM	2555	OG	SER	B	19	63.070	106.843	16.237	1.00	54.17	B
ATOM	2556	C	SER	B	19	60.213	106.155	15.540	1.00	51.20	B
ATOM	2557	O	SER	B	19	60.569	105.165	14.900	1.00	42.62	B
ATOM	2558	N	THR	B	20	59.347	107.041	15.073	1.00	48.91	B
ATOM	2559	CA	THR	B	20	58.706	106.898	13.783	1.00	49.40	B
ATOM	2560	CB	THR	B	20	57.166	107.002	13.991	1.00	52.73	B
ATOM	2561	OG1	THR	B	20	56.483	106.279	12.968	1.00	60.25	B
ATOM	2562	CG2	THR	B	20	56.714	108.456	13.943	1.00	51.71	B
ATOM	2563	C	THR	B	20	59.222	108.022	12.844	1.00	47.48	B
ATOM	2564	O	THR	B	20	59.460	109.147	13.280	1.00	50.56	B
ATOM	2565	N	PRO	B	21	59.427	107.720	11.551	1.00	46.52	B
ATOM	2566	CD	PRO	B	21	59.801	108.745	10.551	1.00	44.33	B
ATOM	2567	CA	PRO	B	21	59.204	106.417	10.909	1.00	46.20	B
ATOM	2568	CB	PRO	B	21	59.137	106.769	9.422	1.00	43.49	B
ATOM	2569	CG	PRO	B	21	60.103	107.918	9.305	1.00	44.19	B
ATOM	2570	C	PRO	B	21	60.342	105.456	11.248	1.00	37.71	B
ATOM	2571	O	PRO	B	21	61.393	105.891	11.674	1.00	38.42	B
ATOM	2572	N	THR	B	22	60.123	104.155	11.067	1.00	40.00	B
ATOM	2573	CA	THR	B	22	61.139	103.150	11.382	1.00	37.29	B
ATOM	2574	CB	THR	B	22	60.521	101.715	11.578	1.00	33.63	B
ATOM	2575	OG1	THR	B	22	59.497	101.719	12.600	1.00	36.55	B
ATOM	2576	CG2	THR	B	22	61.626	100.734	11.963	1.00	29.99	B
ATOM	2577	C	THR	B	22	62.143	103.079	10.221	1.00	35.94	B
ATOM	2578	O	THR	B	22	61.851	102.484	9.183	1.00	33.29	B
ATOM	2579	N	ALA	B	23	63.326	103.663	10.410	1.00	33.77	B
ATOM	2580	CA	ALA	B	23	64.367	103.677	9.380	1.00	30.19	B
ATOM	2581	CB	ALA	B	23	65.314	104.852	9.615	1.00	28.90	B
ATOM	2582	C	ALA	B	23	65.192	102.399	9.300	1.00	30.98	B
ATOM	2583	O	ALA	B	23	65.331	101.693	10.284	1.00	23.97	B

ATOM	2584	N	VAL	B	24	65.736	102.127	8.112	1.00	27.61	B
ATOM	2585	CA	VAL	B	24	66.591	100.982	7.874	1.00	26.92	B
ATOM	2586	CB	VAL	B	24	67.197	101.042	6.460	1.00	29.41	B
ATOM	2587	CG1	VAL	B	24	68.357	100.043	6.326	1.00	28.58	B
ATOM	2588	CG2	VAL	B	24	66.107	100.729	5.430	1.00	26.92	B
ATOM	2589	C	VAL	B	24	67.707	101.091	8.898	1.00	32.79	B
ATOM	2590	O	VAL	B	24	68.266	102.166	9.077	1.00	26.10	B
ATOM	2591	N	GLY	B	25	68.026	100.000	9.586	1.00	28.01	B
ATOM	2592	CA	GLY	B	25	69.070	100.081	10.596	1.00	31.93	B
ATOM	2593	C	GLY	B	25	68.516	100.210	12.007	1.00	34.29	B
ATOM	2594	O	GLY	B	25	69.251	100.080	12.966	1.00	28.44	B
ATOM	2595	N	THR	B	26	67.227	100.486	12.148	1.00	26.99	B
ATOM	2596	CA	THR	B	26	66.650	100.568	13.474	1.00	29.37	B
ATOM	2597	CB	THR	B	26	65.179	100.994	13.403	1.00	30.78	B
ATOM	2598	OG1	THR	B	26	65.111	102.295	12.808	1.00	26.87	B
ATOM	2599	CG2	THR	B	26	64.524	101.000	14.833	1.00	23.56	B
ATOM	2600	C	THR	B	26	66.713	99.183	14.136	1.00	32.07	B
ATOM	2601	O	THR	B	26	66.462	98.171	13.473	1.00	28.44	B
ATOM	2602	N	VAL	B	27	67.056	99.143	15.429	1.00	28.90	B
ATOM	2603	CA	VAL	B	27	67.124	97.891	16.200	1.00	29.71	B
ATOM	2604	CB	VAL	B	27	68.507	97.703	16.858	1.00	36.67	B
ATOM	2605	CG1	VAL	B	27	68.477	96.507	17.808	1.00	31.87	B
ATOM	2606	CG2	VAL	B	27	69.554	97.478	15.793	1.00	32.00	B
ATOM	2607	C	VAL	B	27	66.054	97.946	17.292	1.00	25.09	B
ATOM	2608	O	VAL	B	27	65.961	98.921	18.029	1.00	28.74	B
ATOM	2609	N	ILE	B	28	65.230	96.913	17.349	1.00	28.74	B
ATOM	2610	CA	ILE	B	28	64.126	96.780	18.294	1.00	34.25	B
ATOM	2611	CB	ILE	B	28	62.802	96.400	17.552	1.00	38.10	B
ATOM	2612	CG2	ILE	B	28	61.752	95.929	18.516	1.00	49.78	B
ATOM	2613	CG1	ILE	B	28	62.260	97.598	16.808	1.00	46.71	B
ATOM	2614	CD1	ILE	B	28	62.252	98.826	17.612	1.00	40.93	B
ATOM	2615	C	ILE	B	28	64.491	95.619	19.223	1.00	38.36	B
ATOM	2616	O	ILE	B	28	65.063	94.626	18.769	1.00	29.90	B
ATOM	2617	N	ARG	B	29	64.134	95.724	20.503	1.00	30.42	B
ATOM	2618	CA	ARG	B	29	64.470	94.673	21.458	1.00	32.43	B
ATOM	2619	CB	ARG	B	29	65.468	95.242	22.461	1.00	38.54	B
ATOM	2620	CG	ARG	B	29	66.234	94.231	23.273	1.00	56.74	B
ATOM	2621	CD	ARG	B	29	67.479	94.939	23.821	1.00	68.43	B
ATOM	2622	NE	ARG	B	29	68.210	95.573	22.722	1.00	77.31	B
ATOM	2623	CZ	ARG	B	29	69.134	94.960	21.983	1.00	81.92	B
ATOM	2624	NH1	ARG	B	29	69.454	93.693	22.237	1.00	82.00	B
ATOM	2625	NH2	ARG	B	29	69.723	95.603	20.976	1.00	82.81	B
ATOM	2626	C	ARG	B	29	63.222	94.132	22.168	1.00	26.06	B
ATOM	2627	O	ARG	B	29	62.432	94.884	22.704	1.00	20.11	B
ATOM	2628	N	TYR	B	30	63.032	92.823	22.133	1.00	22.95	B
ATOM	2629	CA	TYR	B	30	61.886	92.206	22.787	1.00	31.30	B
ATOM	2630	CB	TYR	B	30	61.299	91.096	21.905	1.00	28.61	B
ATOM	2631	CG	TYR	B	30	60.647	91.547	20.605	1.00	29.37	B
ATOM	2632	CD1	TYR	B	30	61.389	92.135	19.579	1.00	24.77	B
ATOM	2633	CE1	TYR	B	30	60.781	92.553	18.387	1.00	19.11	B
ATOM	2634	CD2	TYR	B	30	59.282	91.378	20.403	1.00	29.03	B
ATOM	2635	CE2	TYR	B	30	58.674	91.785	19.215	1.00	26.35	B
ATOM	2636	CZ	TYR	B	30	59.429	92.379	18.216	1.00	23.41	B
ATOM	2637	OH	TYR	B	30	58.793	92.836	17.083	1.00	26.05	B
ATOM	2638	C	TYR	B	30	62.340	91.579	24.126	1.00	28.33	B

ATOM	2639	O	TYR	B	30	53.497	91.168	24.283	1.00	24.49	B
ATOM	2640	N	SER	B	31	61.418	91.488	25.067	1.00	26.50	B
ATOM	2641	CA	SER	B	31	61.697	90.903	26.369	1.00	24.95	B
ATOM	2642	CB	SER	B	31	62.304	91.946	27.308	1.00	21.32	B
ATOM	2643	OG	SER	B	31	61.426	93.028	27.483	1.00	26.55	B
ATOM	2644	C	SER	B	31	60.388	90.378	26.954	1.00	29.25	B
ATOM	2645	O	SER	B	31	59.287	90.780	26.529	1.00	22.45	B
ATOM	2646	N	CYS	B	32	60.515	89.484	27.930	1.00	27.99	B
ATOM	2647	CA	CYS	B	32	59.364	88.868	28.606	1.00	32.41	B
ATOM	2648	C	CYS	B	32	59.371	89.122	30.121	1.00	38.37	B
ATOM	2649	O	CYS	B	32	60.431	89.311	30.719	1.00	37.82	B
ATOM	2650	CB	CYS	B	32	59.371	87.347	28.400	1.00	30.70	B
ATOM	2651	SG	CYS	B	32	59.460	86.770	26.677	1.00	32.11	B
ATOM	2652	N	SER	B	33	58.178	89.101	30.717	1.00	51.37	B
ATOM	2653	CA	SER	B	33	57.995	89.265	32.163	1.00	56.15	B
ATOM	2654	CB	SER	B	33	56.544	89.013	32.552	1.00	60.18	B
ATOM	2655	OG	SER	B	33	55.675	89.714	31.672	1.00	66.23	B
ATOM	2656	C	SER	B	33	58.859	88.260	32.894	1.00	57.27	B
ATOM	2657	O	SER	B	33	59.535	87.427	32.274	1.00	60.30	B
ATOM	2658	N	GLY	B	34	58.805	88.290	34.219	1.00	53.29	B
ATOM	2659	CA	GLY	B	34	59.662	87.391	34.976	1.00	47.70	B
ATOM	2660	C	GLY	B	34	59.278	85.922	34.987	1.00	44.48	B
ATOM	2661	O	GLY	B	34	60.129	85.033	35.135	1.00	38.34	B
ATOM	2662	N	THR	B	35	57.993	85.660	34.818	1.00	40.51	B
ATOM	2663	CA	THR	B	35	57.524	84.290	34.860	1.00	40.76	B
ATOM	2664	CB	THR	B	35	56.225	84.239	35.644	1.00	41.73	B
ATOM	2665	OG1	THR	B	35	55.258	85.077	35.014	1.00	48.51	B
ATOM	2666	CG2	THR	B	35	56.468	84.761	37.057	1.00	44.89	B
ATOM	2667	C	THR	B	35	57.369	83.691	33.470	1.00	39.51	B
ATOM	2668	O	THR	B	35	56.786	82.613	33.286	1.00	31.97	B
ATOM	2669	N	PHE	B	36	57.924	84.399	32.491	1.00	35.56	B
ATOM	2670	CA	PHE	B	36	57.873	83.955	31.112	1.00	31.01	B
ATOM	2671	CB	PHE	B	36	57.146	84.967	30.250	1.00	33.05	B
ATOM	2672	CG	PHE	B	36	55.673	84.918	30.396	1.00	35.23	B
ATOM	2673	CD1	PHE	B	36	55.040	85.573	31.444	1.00	35.53	B
ATOM	2674	CD2	PHE	B	36	54.909	84.204	29.483	1.00	31.53	B
ATOM	2675	CE1	PHE	B	36	53.663	85.497	31.570	1.00	37.58	B
ATOM	2676	CE2	PHE	B	36	53.549	84.126	29.604	1.00	32.60	B
ATOM	2677	CZ	PHE	B	36	52.918	84.769	30.638	1.00	32.38	B
ATOM	2678	C	PHE	B	36	59.276	83.798	30.577	1.00	32.83	B
ATOM	2679	O	PHE	B	36	60.212	84.347	31.125	1.00	33.40	B
ATOM	2680	N	ARG	B	37	59.427	83.049	29.498	1.00	30.99	B
ATOM	2681	CA	ARG	B	37	60.741	82.896	28.916	1.00	29.69	B
ATOM	2682	CB	ARG	B	37	61.201	81.458	29.083	1.00	30.62	B
ATOM	2683	CG	ARG	B	37	61.442	81.072	30.541	1.00	35.61	B
ATOM	2684	CD	ARG	B	37	62.492	81.992	31.177	1.00	39.39	B
ATOM	2685	NE	ARG	B	37	62.303	82.044	32.629	1.00	49.28	B
ATOM	2686	CZ	ARG	B	37	62.847	81.168	33.451	1.00	47.41	B
ATOM	2687	NH1	ARG	B	37	63.614	80.212	32.947	1.00	53.00	B
ATOM	2688	NH2	ARG	B	37	62.602	81.223	34.751	1.00	44.10	B
ATOM	2689	C	ARG	B	37	60.713	83.280	27.439	1.00	32.05	B
ATOM	2690	O	ARG	B	37	59.809	82.874	26.700	1.00	25.63	B
ATOM	2691	N	LEU	B	38	61.706	84.050	27.011	1.00	23.96	B
ATOM	2692	CA	LEU	B	38	61.802	84.470	25.621	1.00	30.62	B
ATOM	2693	CB	LEU	B	38	62.655	85.738	25.508	1.00	23.25	B

ATOM	2694	CG	LEU	B	38	62.739	86.365	24.105	1.00	28.16	B
ATOM	2695	CD1	LEU	B	38	61.376	86.948	23.659	1.00	20.01	B
ATOM	2696	CD2	LEU	B	38	63.753	87.486	24.132	1.00	32.19	B
ATOM	2697	C	LEU	B	38	62.386	83.361	24.745	1.00	27.63	B
ATOM	2698	O	LEU	B	38	63.447	82.793	25.036	1.00	27.98	B
ATOM	2699	N	ILE	B	39	61.651	83.017	23.691	1.00	30.18	B
ATOM	2700	CA	ILE	B	39	62.073	81.983	22.743	1.00	27.37	B
ATOM	2701	CB	ILE	B	39	60.940	80.959	22.492	1.00	30.75	B
ATOM	2702	CG2	ILE	B	39	61.438	79.878	21.538	1.00	29.27	B
ATOM	2703	CG1	ILE	B	39	60.455	80.359	23.822	1.00	30.90	B
ATOM	2704	CD1	ILE	B	39	61.491	79.535	24.559	1.00	26.44	B
ATOM	2705	C	ILE	B	39	62.403	82.668	21.418	1.00	29.53	B
ATOM	2706	O	ILE	B	39	61.510	83.256	20.797	1.00	24.87	B
ATOM	2707	N	GLY	B	40	63.676	82.609	20.998	1.00	21.97	B
ATOM	2708	CA	GLY	B	40	64.084	83.239	19.751	1.00	23.62	B
ATOM	2709	C	GLY	B	40	64.957	84.450	19.975	1.00	22.85	B
ATOM	2710	O	GLY	B	40	65.065	84.921	21.104	1.00	21.42	B
ATOM	2711	N	GLU	B	41	65.592	84.958	18.925	1.00	27.33	B
ATOM	2712	CA	GLU	B	41	66.472	86.133	19.065	1.00	29.50	B
ATOM	2713	CB	GLU	B	41	67.138	86.471	17.730	1.00	33.78	B
ATOM	2714	CG	GLU	B	41	68.634	86.193	17.721	1.00	52.17	B
ATOM	2715	CD	GLU	B	41	69.411	87.123	18.648	1.00	57.74	B
ATOM	2716	OE1	GLU	B	41	70.414	86.641	19.231	1.00	66.30	B
ATOM	2717	OE2	GLU	B	41	69.034	88.326	18.791	1.00	53.76	B
ATOM	2718	C	GLU	B	41	65.667	87.333	19.541	1.00	30.40	B
ATOM	2719	O	GLU	B	41	64.601	87.619	18.995	1.00	27.22	B
ATOM	2720	N	LYS	B	42	66.197	88.049	20.528	1.00	27.86	B
ATOM	2721	CA	LYS	B	42	65.538	89.215	21.135	1.00	32.03	B
ATOM	2722	CB	LYS	B	42	66.171	89.495	22.504	1.00	37.19	B
ATOM	2723	CG	LYS	B	42	67.610	89.990	22.379	1.00	43.78	B
ATOM	2724	CD	LYS	B	42	68.196	90.536	23.674	1.00	54.68	B
ATOM	2725	CE	LYS	B	42	68.055	89.538	24.812	1.00	62.51	B
ATOM	2726	NZ	LYS	B	42	68.438	88.139	24.443	1.00	69.20	B
ATOM	2727	C	LYS	B	42	63.586	90.530	20.331	1.00	32.32	B
ATOM	2728	O	LYS	B	42	64.771	91.432	20.555	1.00	27.61	B
ATOM	2729	N	SER	B	43	66.547	90.680	19.422	1.00	28.99	B
ATOM	2730	CA	SER	B	43	66.611	91.946	18.672	1.00	33.61	B
ATOM	2731	CB	SER	B	43	68.012	92.565	18.722	1.00	29.97	B
ATOM	2732	OG	SER	B	43	68.478	92.606	20.047	1.00	47.21	B
ATOM	2733	C	SER	B	43	66.273	91.770	17.224	1.00	28.57	B
ATOM	2734	O	SER	B	43	66.765	90.841	16.588	1.00	32.11	B
ATOM	2735	N	LEU	B	44	65.443	92.661	16.697	1.00	26.09	B
ATOM	2736	CA	LEU	B	44	65.127	92.607	15.280	1.00	25.34	B
ATOM	2737	CB	LEU	B	44	63.620	92.609	14.987	1.00	21.75	B
ATOM	2738	CG	LEU	B	44	62.803	91.642	15.833	1.00	23.26	B
ATOM	2739	CD1	LEU	B	44	61.455	91.487	14.626	1.00	24.66	B
ATOM	2740	CD2	LEU	B	44	63.227	90.293	15.976	1.00	19.72	B
ATOM	2741	C	LEU	B	44	65.738	93.863	14.694	1.00	27.39	B
ATOM	2742	O	LEU	B	44	65.759	94.919	15.334	1.00	29.07	B
ATOM	2743	N	LEU	B	45	66.201	93.740	13.456	1.00	26.79	B
ATOM	2744	CA	LEU	B	45	66.854	94.812	12.727	1.00	26.17	B
ATOM	2745	CB	LEU	B	45	68.202	94.303	12.213	1.00	25.36	B
ATOM	2746	CG	LEU	B	45	69.343	95.281	11.950	1.00	35.90	B
ATOM	2747	CD1	LEU	B	45	70.263	94.668	10.905	1.00	31.78	B
ATOM	2748	CD2	LEU	B	45	68.853	96.627	11.519	1.00	39.62	B

ATOM	2749	C	LEU	B	45	66.016	95.198	11.516	1.00	25.11	B
ATOM	2750	O	LEU	B	45	65.568	94.320	10.761	1.00	20.94	B
ATOM	2751	N	CYS	B	46	65.803	96.487	11.298	1.00	24.85	B
ATOM	2752	CA	CYS	B	46	65.057	96.837	10.097	1.00	22.87	B
ATOM	2753	C	CYS	B	46	66.106	96.897	8.976	1.00	29.24	B
ATOM	2754	O	CYS	B	46	67.099	97.601	9.051	1.00	28.50	B
ATOM	2755	CB	CYS	B	46	64.446	98.284	10.261	1.00	26.50	B
ATOM	2756	SG	CYS	B	46	63.677	98.900	8.705	1.00	27.31	B
ATOM	2757	N	ILE	B	47	65.877	96.106	7.943	1.00	24.65	B
ATOM	2758	CA	ILE	B	47	66.817	95.991	6.842	1.00	28.64	B
ATOM	2759	CB	ILE	B	47	67.412	94.572	6.871	1.00	30.17	B
ATOM	2760	CG2	ILE	B	47	68.114	94.258	5.601	1.00	42.28	B
ATOM	2761	CG1	ILE	B	47	68.341	94.458	8.070	1.00	40.16	B
ATOM	2762	CD1	ILE	B	47	69.121	93.190	8.107	1.00	53.27	B
ATOM	2763	C	ILE	B	47	66.098	96.188	5.504	1.00	28.32	B
ATOM	2764	O	ILE	B	47	64.874	96.332	5.466	1.00	24.72	B
ATOM	2765	N	THR	B	48	66.853	96.238	4.413	1.00	24.30	B
ATOM	2766	CA	THR	B	48	66.236	96.267	3.091	1.00	27.24	B
ATOM	2767	CB	THR	B	48	66.215	97.672	2.405	1.00	31.04	B
ATOM	2768	OG1	THR	B	48	65.632	97.534	1.090	1.00	26.58	B
ATOM	2769	CG2	THR	B	48	67.627	98.250	2.271	1.00	23.59	B
ATOM	2770	C	THR	B	48	67.048	95.280	2.254	1.00	26.55	B
ATOM	2771	O	THR	B	48	68.276	95.371	2.173	1.00	27.30	B
ATOM	2772	N	LYS	B	49	66.370	94.295	1.688	1.00	24.39	B
ATOM	2773	CA	LYS	B	49	67.031	93.309	0.837	1.00	25.65	B
ATOM	2774	CB	LYS	B	49	66.323	91.943	0.940	1.00	27.44	B
ATOM	2775	CG	LYS	B	49	66.358	91.351	2.368	1.00	36.21	B
ATOM	2776	CD	LYS	B	49	67.171	90.103	2.479	1.00	40.52	B
ATOM	2777	CE	LYS	B	49	68.570	90.294	3.025	1.00	41.63	B
ATOM	2778	NZ	LYS	B	49	69.314	89.069	2.403	1.00	46.47	B
ATOM	2779	C	LYS	B	49	67.041	93.752	-0.632	1.00	33.01	B
ATOM	2780	O	LYS	B	49	67.987	93.450	-1.353	1.00	28.70	B
ATOM	2781	N	ASP	B	50	65.994	94.451	-1.083	1.00	26.02	B
ATOM	2782	CA	ASP	B	50	65.933	94.859	-2.495	1.00	29.77	B
ATOM	2783	CB	ASP	B	50	64.575	94.503	-3.108	1.00	28.99	B
ATOM	2784	CG	ASP	B	50	63.439	95.221	-2.440	1.00	26.54	B
ATOM	2785	OD1	ASP	B	50	63.720	95.043	-1.562	1.00	25.74	B
ATOM	2786	OD2	ASP	B	50	62.262	94.969	-0.779	1.00	32.42	B
ATOM	2787	C	ASP	B	50	66.200	96.327	-2.744	1.00	30.62	B
ATOM	2788	O	ASP	B	50	66.037	96.794	-3.858	1.00	24.13	B
ATOM	2789	N	LYS	B	51	66.610	97.050	-1.709	1.00	27.94	B
ATOM	2790	CA	LYS	B	51	66.889	98.473	-1.824	1.00	31.18	B
ATOM	2791	CB	LYS	B	51	68.014	98.742	-2.819	1.00	34.46	B
ATOM	2792	CG	LYS	B	51	69.381	98.355	-2.297	1.00	41.85	B
ATOM	2793	CD	LYS	B	51	70.447	98.960	-3.175	1.00	49.97	B
ATOM	2794	CE	LYS	B	51	71.826	98.869	-2.561	1.00	59.90	B
ATOM	2795	NZ	LYS	B	51	72.754	99.713	3.366	1.00	67.70	B
ATOM	2796	C	LYS	B	51	65.666	99.305	-2.186	1.00	30.87	B
ATOM	2797	O	LYS	B	51	65.786	100.430	-2.634	1.00	28.68	B
ATOM	2798	N	VAL	B	52	64.483	98.743	-1.992	1.00	26.95	B
ATOM	2799	CA	VAL	B	52	63.263	99.501	-2.231	1.00	26.37	B
ATOM	2800	CB	VAL	B	52	62.456	98.945	-3.402	1.00	27.69	B
ATOM	2801	CG1	VAL	B	52	61.123	99.695	-3.511	1.00	32.70	B
ATOM	2802	CG2	VAL	B	52	63.236	99.113	-4.679	1.00	32.13	B
ATOM	2803	C	VAL	B	52	62.375	99.437	-1.000	1.00	30.79	B

ATOM	2804	O	VAL	B	52	61.949	100.461	-0.491	1.00	26.76	B
ATOM	2805	N	ASP	B	53	62.102	98.232	-0.512	1.00	26.86	B
ATOM	2806	CA	ASP	B	53	61.210	98.074	0.642	1.00	26.94	B
ATOM	2807	CB	ASP	B	53	60.156	96.999	0.318	1.00	42.02	B
ATOM	2808	CG	ASP	B	53	59.285	97.356	-0.871	1.00	53.53	B
ATOM	2809	OD1	ASP	B	53	58.878	98.540	-0.943	1.00	63.13	B
ATOM	2810	OD2	ASP	B	53	58.964	96.476	-1.727	1.00	64.13	B
ATOM	2811	C	ASP	B	53	62.006	97.651	1.888	1.00	25.00	B
ATOM	2812	O	ASP	B	53	63.063	97.038	1.773	1.00	22.23	B
ATOM	2813	N	GLY	B	54	61.490	97.959	3.072	1.00	20.64	B
ATOM	2814	CA	GLY	B	54	62.170	97.578	4.293	1.00	24.10	B
ATOM	2815	C	GLY	B	54	61.441	96.397	4.919	1.00	25.17	B
ATOM	2816	O	GLY	B	54	60.237	96.266	4.728	1.00	25.23	B
ATOM	2817	N	THR	B	55	62.169	95.517	5.605	1.00	23.87	B
ATOM	2818	CA	THR	B	55	61.589	94.373	6.318	1.00	20.36	B
ATOM	2819	CB	THR	B	55	61.679	93.051	5.518	1.00	27.74	B
ATOM	2820	OG1	THR	B	55	61.052	92.004	6.267	1.00	24.11	B
ATOM	2821	CG2	THR	B	55	63.151	92.669	5.312	1.00	21.92	B
ATOM	2822	C	THR	B	55	62.371	94.156	7.600	1.00	22.54	B
ATOM	2823	O	THR	B	55	63.535	94.526	7.675	1.00	24.57	B
ATOM	2824	N	TRP	B	56	61.743	93.589	8.624	1.00	23.11	B
ATOM	2825	CA	TRP	B	56	62.513	93.285	9.827	1.00	25.54	B
ATOM	2826	CB	TRP	B	56	61.580	92.954	10.988	1.00	23.18	B
ATOM	2827	CG	TRP	B	56	60.874	94.202	11.400	1.00	19.51	B
ATOM	2828	CD2	TRP	B	56	61.456	95.282	12.147	1.00	21.91	B
ATOM	2829	CE2	TRP	B	56	60.473	96.302	12.247	1.00	26.89	B
ATOM	2830	CE3	TRP	B	56	62.722	95.491	12.729	1.00	25.30	B
ATOM	2831	CD1	TRP	B	56	59.595	94.578	11.119	1.00	21.93	B
ATOM	2832	NE1	TRP	B	56	59.343	95.849	11.617	1.00	21.49	B
ATOM	2833	CZ2	TRP	B	56	60.713	97.521	12.895	1.00	26.71	B
ATOM	2834	CZ3	TRP	B	56	62.963	96.706	13.330	1.00	29.35	B
ATOM	2835	CH2	TRP	B	56	61.957	97.706	13.451	1.00	28.96	B
ATOM	2836	C	TRP	B	56	63.335	92.075	9.384	1.00	28.11	B
ATOM	2837	O	TRP	B	56	62.882	91.296	8.535	1.00	23.54	B
ATOM	2838	N	ASP	B	57	64.535	91.909	9.926	1.00	20.44	B
ATOM	2839	CA	ASP	B	57	65.401	90.812	9.470	1.00	25.81	B
ATOM	2840	CB	ASP	B	57	66.885	91.113	9.761	1.00	30.15	B
ATOM	2841	CG	ASP	B	57	67.234	91.045	11.255	1.00	35.84	B
ATOM	2842	OD1	ASP	B	57	66.319	91.161	12.102	1.00	23.31	B
ATOM	2843	OD2	ASP	B	57	68.443	90.889	11.581	1.00	41.06	B
ATOM	2844	C	ASP	B	57	65.058	89.433	9.963	1.00	26.11	B
ATOM	2845	O	ASP	B	57	65.634	88.455	9.486	1.00	28.90	B
ATOM	2846	N	LYS	B	58	64.114	89.336	10.896	1.00	29.91	B
ATOM	2847	CA	LYS	B	58	63.687	88.032	11.411	1.00	27.97	B
ATOM	2848	CB	LYS	B	58	64.697	87.491	12.443	1.00	30.61	B
ATOM	2849	CG	LYS	B	58	64.884	88.378	13.650	1.00	38.23	B
ATOM	2850	CD	LYS	B	58	65.966	87.831	14.618	1.00	41.02	B
ATOM	2851	CE	LYS	B	58	67.406	88.063	14.115	1.00	37.73	B
ATOM	2852	NZ	LYS	B	58	67.830	89.511	14.219	1.00	29.19	B
ATOM	2853	C	LYS	B	58	62.319	88.105	12.045	1.00	22.71	B
ATOM	2854	O	LYS	B	58	61.795	89.188	12.311	1.00	26.33	B
ATOM	2855	N	PRO	B	59	61.700	86.947	12.292	1.00	25.99	B
ATOM	2856	CD	PRO	B	59	62.084	85.584	11.885	1.00	24.09	B
ATOM	2857	CA	PRO	B	59	60.367	86.972	12.919	1.00	22.11	B
ATOM	2858	CB	PRO	B	59	59.902	85.515	12.845	1.00	26.86	B

ATOM	2859	CG	PRO	B	59	60.730	84.913	11.746	1.00	29.91	B
ATOM	2860	C	PRO	B	59	60.509	87.419	14.369	1.00	30.21	B
ATOM	2861	O	PRO	B	59	61.593	87.307	14.968	1.00	28.15	B
ATOM	2862	N	ALA	B	60	59.433	87.924	14.951	1.00	25.43	B
ATOM	2863	CA	ALA	B	60	59.516	88.330	16.339	1.00	26.37	B
ATOM	2864	CB	ALA	B	60	58.260	89.089	16.742	1.00	26.63	B
ATOM	2865	C	ALA	B	60	59.644	87.085	17.223	1.00	21.31	B
ATOM	2866	O	ALA	B	60	59.104	86.068	16.914	1.00	22.47	B
ATOM	2867	N	PRO	B	61	60.358	87.173	18.350	1.00	23.37	B
ATOM	2868	CD	PRO	B	61	61.134	88.320	18.870	1.00	22.24	B
ATOM	2869	CA	PRO	B	61	60.476	86.007	19.227	1.00	19.99	B
ATOM	2870	CB	PRO	B	61	61.650	86.386	20.130	1.00	21.18	B
ATOM	2871	CG	PRO	B	61	61.458	87.876	20.314	1.00	22.73	B
ATOM	2872	C	PRO	B	61	59.151	85.933	20.024	1.00	27.42	B
ATOM	2873	O	PRO	B	61	58.314	86.831	19.903	1.00	27.48	B
ATOM	2874	N	LYS	B	62	58.960	84.893	20.834	1.00	21.73	B
ATOM	2875	CA	LYS	B	62	57.737	84.770	21.648	1.00	26.90	B
ATOM	2876	CB	LYS	B	62	56.880	83.576	21.187	1.00	32.90	B
ATOM	2877	CG	LYS	B	62	56.318	83.743	19.779	1.00	39.12	B
ATOM	2878	CD	LYS	B	62	55.638	82.502	19.258	1.00	48.29	B
ATOM	2879	CE	LYS	B	62	55.142	82.741	17.828	1.00	54.55	B
ATOM	2880	NZ	LYS	B	62	54.620	81.478	17.213	1.00	59.87	B
ATOM	2881	C	LYS	B	62	58.050	84.601	23.133	1.00	30.68	B
ATOM	2882	O	LYS	B	62	59.190	84.287	23.528	1.00	24.62	B
ATOM	2883	N	CYS	B	63	57.039	84.843	23.958	1.00	25.15	B
ATOM	2884	CA	CYS	B	63	57.171	84.675	25.405	1.00	27.27	B
ATOM	2885	C	CYS	B	63	56.314	83.481	25.792	1.00	30.43	B
ATOM	2886	O	CYS	B	63	55.111	83.454	25.515	1.00	30.82	B
ATOM	2887	CB	CYS	B	63	56.646	85.903	26.149	1.00	25.60	B
ATOM	2888	SG	CYS	B	63	57.682	87.384	25.922	1.00	31.81	B
ATOM	2889	N	GLU	B	64	56.934	82.486	26.414	1.00	29.14	B
ATOM	2890	CA	GLU	B	64	56.220	81.297	26.871	1.00	27.87	B
ATOM	2891	CB	GLU	B	64	56.938	80.043	26.393	1.00	22.54	B
ATOM	2892	CG	GLU	B	64	56.839	79.836	24.884	1.00	30.23	B
ATOM	2893	CD	GLU	B	64	57.364	78.472	24.471	1.00	25.42	B
ATOM	2894	OE1	GLU	B	64	58.146	77.879	25.221	1.00	28.63	B
ATOM	2895	OE2	GLU	B	64	56.993	77.994	23.396	1.00	24.45	B
ATOM	2896	C	GLU	B	64	56.172	81.301	28.394	1.00	27.43	B
ATOM	2897	O	GLU	B	64	57.189	81.564	29.036	1.00	28.45	B
ATOM	2898	N	TYR	B	65	55.003	81.039	28.981	1.00	30.82	B
ATOM	2899	CA	TYR	B	65	54.898	81.016	30.449	1.00	26.71	B
ATOM	2900	CB	TYR	B	65	53.474	80.638	30.881	1.00	24.67	B
ATOM	2901	CG	TYR	B	65	53.222	80.754	32.382	1.00	30.61	B
ATOM	2902	CD1	TYR	B	65	53.558	81.915	33.078	1.00	37.96	B
ATOM	2903	CE1	TYR	B	65	53.369	82.013	34.464	1.00	37.10	B
ATOM	2904	CD2	TYR	B	65	52.681	79.689	33.102	1.00	29.91	B
ATOM	2905	CE2	TYR	B	65	52.481	79.765	34.477	1.00	32.64	B
ATOM	2906	CZ	TYR	B	65	52.829	80.927	35.149	1.00	38.91	B
ATOM	2907	OH	TYR	B	65	52.653	81.014	36.510	1.00	40.82	B
ATOM	2908	C	TYR	B	65	55.931	79.969	30.908	1.00	26.37	B
ATOM	2909	O	TYR	B	65	56.022	78.891	30.339	1.00	27.39	B
ATOM	2910	N	PHE	B	66	56.722	80.290	31.924	1.00	30.93	B
ATOM	2911	CA	PHE	B	66	57.770	79.381	32.362	1.00	29.14	B
ATOM	2912	CB	PHE	B	66	58.611	80.060	33.455	1.00	27.56	B
ATOM	2913	CG	PHE	B	66	59.743	79.210	33.998	1.00	28.67	B

ATOM	2914	CD1	PHE	B	65	60.632	78.559	33.139	1.00	33.68	B
ATOM	2915	CD2	PHE	B	66	59.907	79.055	35.371	1.00	30.48	B
ATOM	2916	CE1	PHE	B	66	61.669	77.763	33.648	1.00	35.23	B
ATOM	2917	CE2	PHE	B	66	60.931	78.267	35.895	1.00	26.93	B
ATOM	2918	CZ	PHE	B	66	61.816	77.618	35.041	1.00	31.25	B
ATOM	2919	C	PHE	B	66	57.283	78.013	32.844	1.00	32.09	B
ATOM	2920	O	PHE	B	66	56.382	77.924	33.671	1.00	31.84	B
ATOM	2921	N	ASN	B	67	57.882	76.956	32.312	1.00	28.91	B
ATOM	2922	CA	ASN	B	67	57.553	75.591	32.727	1.00	31.14	B
ATOM	2923	CB	ASN	B	67	57.124	74.763	31.524	1.00	32.40	B
ATOM	2924	CG	ASN	B	67	56.635	73.368	31.903	1.00	37.56	B
ATOM	2925	OD1	ASN	B	67	57.193	72.701	32.784	1.00	33.77	B
ATOM	2926	ND2	ASN	B	67	55.589	72.914	31.218	1.00	40.31	B
ATOM	2927	C	ASN	B	67	58.844	75.009	33.318	1.00	30.31	B
ATOM	2928	O	ASN	B	67	59.719	74.551	32.577	1.00	26.39	B
ATOM	2929	N	LYS	B	68	58.960	75.038	34.644	1.00	28.27	B
ATOM	2930	CA	LYS	B	68	60.148	74.535	35.329	1.00	29.00	B
ATOM	2931	CB	LYS	B	68	60.041	74.792	36.843	1.00	35.08	B
ATOM	2932	CG	LYS	B	68	58.984	73.906	37.518	1.00	41.56	B
ATOM	2933	CD	LYS	B	68	59.179	73.778	39.031	1.00	52.33	B
ATOM	2934	CE	LYS	B	68	58.907	75.077	39.764	1.00	54.82	B
ATOM	2935	NZ	LYS	B	68	58.896	74.891	41.250	1.00	58.88	B
ATOM	2936	C	LYS	B	68	60.398	73.039	35.087	1.00	32.74	B
ATOM	2937	O	LYS	B	68	61.507	72.556	35.318	1.00	32.92	B
ATOM	2938	N	TYR	B	69	59.389	72.305	34.611	1.00	33.19	B
ATOM	2939	CA	TYR	B	69	59.559	70.867	34.354	1.00	25.62	B
ATOM	2940	CB	TYR	B	69	58.259	70.096	34.687	1.00	30.97	B
ATOM	2941	CG	TYR	B	69	57.801	70.349	36.107	1.00	30.82	B
ATOM	2942	CD1	TYR	B	69	56.774	71.266	36.378	1.00	28.48	B
ATOM	2943	CE1	TYR	B	69	56.444	71.623	37.697	1.00	31.73	B
ATOM	2944	CD2	TYR	B	69	58.486	69.776	37.192	1.00	31.64	B
ATOM	2945	CE2	TYR	B	69	58.174	70.118	38.507	1.00	38.99	B
ATOM	2946	CZ	TYR	B	69	57.153	71.053	38.756	1.00	39.94	B
ATOM	2947	OH	TYR	B	69	56.901	71.467	40.048	1.00	41.68	B
ATOM	2948	C	TYR	B	69	60.029	70.516	32.955	1.00	31.61	B
ATOM	2949	O	TYR	B	69	60.549	69.414	32.722	1.00	31.53	B
ATOM	2950	N	SER	B	70	59.889	71.447	32.017	1.00	29.13	B
ATOM	2951	CA	SER	B	70	60.328	71.162	30.649	1.00	31.79	B
ATOM	2952	CB	SER	B	70	59.926	72.310	29.708	1.00	27.84	B
ATOM	2953	OG	SER	B	70	58.524	72.534	29.725	1.00	38.42	B
ATOM	2954	C	SER	B	70	61.849	70.949	30.544	1.00	34.24	B
ATOM	2955	O	SER	B	70	62.624	71.534	31.296	1.00	31.38	B
ATOM	2956	N	SER	B	71	62.261	70.097	29.613	1.00	33.64	B
ATOM	2957	CA	SER	B	71	63.676	69.832	29.351	1.00	36.09	B
ATOM	2958	CB	SER	B	71	64.265	68.809	30.324	1.00	39.34	B
ATOM	2959	OG	SER	B	71	63.823	67.519	30.007	1.00	41.01	B
ATOM	2960	C	SER	B	71	63.790	69.308	27.907	1.00	41.17	B
ATOM	2961	O	SER	B	71	62.959	68.520	27.432	1.00	41.90	B
ATOM	2962	N	CYS	B	72	64.805	69.766	27.195	1.00	32.35	B
ATOM	2963	CA	CYS	B	72	64.970	69.351	25.816	1.00	36.35	B
ATOM	2964	C	CYS	B	72	66.139	68.393	25.722	1.00	36.24	B
ATOM	2965	O	CYS	B	72	67.089	68.472	26.503	1.00	34.41	B
ATOM	2966	CB	CYS	B	72	65.205	70.586	24.920	1.00	26.09	B
ATOM	2967	SG	CYS	B	72	63.836	71.795	24.962	1.00	32.64	B
ATOM	2968	N	PRO	B	73	66.069	67.453	24.779	1.00	35.65	B

ATOM	2969	CD	PRO	B	73	64.958	67.148	23.867	1.00	38.10	B
ATOM	2970	CA	PRO	B	73	67.157	66.494	24.617	1.00	35.61	B
ATOM	2971	CB	PRO	B	73	66.567	65.461	23.661	1.00	35.75	B
ATOM	2972	CG	PRO	B	73	65.662	66.314	22.806	1.00	40.23	B
ATOM	2973	C	PRO	B	73	68.355	67.203	24.011	1.00	37.18	B
ATOM	2974	O	PRO	B	73	68.225	68.277	23.427	1.00	31.86	B
ATOM	2975	N	GLU	B	74	69.521	66.595	24.151	1.00	30.08	B
ATOM	2976	CA	GLU	B	74	70.726	67.168	23.594	1.00	36.66	B
ATOM	2977	CB	GLU	B	74	71.904	66.221	23.830	1.00	40.69	B
ATOM	2978	CG	GLU	B	74	73.123	66.500	22.972	1.00	55.61	B
ATOM	2979	CD	GLU	B	74	74.357	66.847	23.791	1.00	65.33	B
ATOM	2980	OE1	GLU	B	74	75.476	66.535	23.311	1.00	68.86	B
ATOM	2981	OE2	GLU	B	74	74.214	67.432	24.899	1.00	67.56	B
ATOM	2982	C	GLU	B	74	70.526	67.411	22.099	1.00	31.83	B
ATOM	2983	O	GLU	B	74	70.179	66.517	21.347	1.00	34.92	B
ATOM	2984	N	PRO	B	75	70.743	68.639	21.648	1.00	29.85	B
ATOM	2985	CD	PRO	B	75	71.019	69.851	22.431	1.00	29.21	B
ATOM	2986	CA	PRO	B	75	70.573	68.944	20.227	1.00	31.16	B
ATOM	2987	CB	PRO	B	75	70.349	70.441	20.235	1.00	30.77	B
ATOM	2988	CG	PRO	B	75	71.310	70.872	21.362	1.00	28.27	B
ATOM	2989	C	PRO	B	75	71.855	68.552	19.507	1.00	37.41	B
ATOM	2990	O	PRO	B	75	72.949	68.998	19.877	1.00	35.98	B
ATOM	2991	N	ILE	B	76	71.728	67.726	18.474	1.00	37.41	B
ATOM	2992	CA	ILE	B	76	72.904	67.277	17.757	1.00	41.40	B
ATOM	2993	CB	ILE	B	76	73.069	65.755	17.912	1.00	47.80	B
ATOM	2994	CG2	ILE	B	76	74.385	65.302	17.272	1.00	48.99	B
ATOM	2995	CG1	ILE	B	76	73.078	65.396	19.404	1.00	48.44	B
ATOM	2996	CD1	ILE	B	76	72.926	63.918	19.671	1.00	55.08	B
ATOM	2997	C	ILE	B	76	72.874	67.654	16.294	1.00	38.62	B
ATOM	2998	O	ILE	B	76	71.874	67.480	15.625	1.00	39.69	B
ATOM	2999	N	VAL	B	77	73.984	68.195	15.813	1.00	36.89	B
ATOM	3000	CA	VAL	B	77	74.107	68.610	14.433	1.00	38.30	B
ATOM	3001	CB	VAL	B	77	74.290	70.119	14.331	1.00	39.19	B
ATOM	3002	CG1	VAL	B	77	74.483	70.519	12.871	1.00	39.16	B
ATOM	3003	CG2	VAL	B	77	73.081	70.826	14.946	1.00	40.99	B
ATOM	3004	C	VAL	B	77	75.307	67.939	13.761	1.00	40.36	B
ATOM	3005	O	VAL	B	77	76.457	68.351	13.948	1.00	41.17	B
ATOM	3006	N	PRO	B	78	75.057	66.893	12.966	1.00	40.75	B
ATOM	3007	CD	PRO	B	78	73.785	66.267	12.590	1.00	37.39	B
ATOM	3008	CA	PRO	B	78	76.183	66.228	12.303	1.00	40.96	B
ATOM	3009	CB	PRO	B	78	75.506	65.195	11.412	1.00	41.91	B
ATOM	3010	CG	PRO	B	78	74.119	65.745	11.229	1.00	45.49	B
ATOM	3011	C	PRO	B	78	76.997	67.232	11.525	1.00	37.80	B
ATOM	3012	O	PRO	B	78	76.447	68.140	10.913	1.00	37.38	B
ATOM	3013	N	GLY	B	79	78.312	67.083	11.590	1.00	32.94	B
ATOM	3014	CA	GLY	B	79	79.186	68.002	10.900	1.00	36.40	B
ATOM	3015	C	GLY	B	79	79.427	69.261	11.712	1.00	34.31	B
ATOM	3016	O	GLY	B	79	80.209	70.109	11.304	1.00	42.13	B
ATOM	3017	N	GLY	B	80	78.760	69.404	12.855	1.00	36.96	B
ATOM	3018	CA	GLY	B	80	78.960	70.608	13.664	1.00	39.25	B
ATOM	3019	C	GLY	B	80	79.072	70.348	15.164	1.00	35.08	B
ATOM	3020	O	GLY	B	80	78.394	69.202	15.609	1.00	40.28	B
ATOM	3021	N	TYR	B	81	79.225	71.410	15.953	1.00	37.65	B
ATOM	3022	CA	TYR	B	81	79.345	71.271	17.408	1.00	33.04	B
ATOM	3023	CB	TYR	B	81	80.800	71.019	17.799	1.00	29.39	B

ATOM	3024	CG	TYR	B	81	81.745	72.112	17.331	1.00	31.26	B
ATOM	3025	CD1	TYR	B	81	82.169	73.116	18.199	1.00	28.35	B
ATOM	3026	CE1	TYR	B	81	82.992	74.143	17.766	1.00	28.17	B
ATOM	3027	CD2	TYR	B	81	82.181	72.163	16.004	1.00	28.62	B
ATOM	3028	CE2	TYR	B	81	83.006	73.183	15.559	1.00	31.47	B
ATOM	3029	CZ	TYR	B	81	83.401	74.174	16.449	1.00	30.40	B
ATOM	3030	OH	TYR	B	81	84.172	75.207	16.012	1.00	32.87	B
ATOM	3031	C	TYR	B	81	78.847	72.536	18.095	1.00	33.96	B
ATOM	3032	O	TYR	B	81	78.696	73.581	17.454	1.00	30.79	B
ATOM	3033	N	LYS	B	82	78.600	72.431	19.398	1.00	23.56	B
ATOM	3034	CA	LYS	B	82	78.114	73.557	20.195	1.00	29.94	B
ATOM	3035	CB	LYS	B	82	77.348	73.034	21.428	1.00	25.29	B
ATOM	3036	CG	LYS	B	82	76.140	72.144	21.057	1.00	27.67	B
ATOM	3037	CD	LYS	B	82	75.335	71.652	22.266	1.00	33.47	B
ATOM	3038	CE	LYS	B	82	76.215	71.041	23.365	1.00	44.83	B
ATOM	3039	NZ	LYS	B	82	77.091	69.944	22.837	1.00	45.24	B
ATOM	3040	C	LYS	B	82	79.205	74.526	20.629	1.00	29.85	B
ATOM	3041	O	LYS	B	82	80.270	74.110	21.099	1.00	31.44	B
ATOM	3042	N	ILE	B	83	78.980	75.822	20.428	1.00	25.93	B
ATOM	3043	CA	ILE	B	83	79.959	76.795	20.887	1.00	21.30	B
ATOM	3044	CB	ILE	B	83	80.449	77.771	19.800	1.00	29.03	B
ATOM	3045	CG2	ILE	B	83	81.296	77.004	18.799	1.00	23.68	B
ATOM	3046	CG1	ILE	B	83	79.278	78.514	19.155	1.00	24.89	B
ATOM	3047	CD1	ILE	B	83	79.722	79.571	18.148	1.00	27.44	B
ATOM	3048	C	ILE	B	83	79.362	77.581	22.027	1.00	26.62	B
ATOM	3049	O	ILE	B	83	80.038	78.408	22.636	1.00	32.15	B
ATOM	3050	N	ARG	B	84	78.092	77.330	22.324	1.00	24.60	B
ATOM	3051	CA	ARG	B	84	77.471	77.981	23.469	1.00	25.74	B
ATOM	3052	CB	ARG	B	84	77.047	79.396	23.131	1.00	34.80	B
ATOM	3053	CG	ARG	B	84	76.583	80.160	24.348	1.00	45.89	B
ATOM	3054	CD	ARG	B	84	76.518	81.629	24.027	1.00	56.25	B
ATOM	3055	NE	ARG	B	84	77.801	82.302	24.217	1.00	62.31	B
ATOM	3056	CZ	ARG	B	84	78.276	82.707	25.397	1.00	64.61	B
ATOM	3057	NH1	ARG	B	84	77.581	82.496	26.512	1.00	65.21	B
ATOM	3058	NH2	ARG	B	84	79.421	83.386	25.454	1.00	61.85	B
ATOM	3059	C	ARG	B	84	76.278	77.199	23.984	1.00	27.61	B
ATOM	3060	O	ARG	B	84	75.487	76.687	23.189	1.00	24.27	B
ATOM	3061	N	GLY	B	85	76.166	77.105	25.314	1.00	25.11	B
ATOM	3062	CA	GLY	B	85	75.074	76.374	25.959	1.00	23.64	B
ATOM	3063	C	GLY	B	85	75.394	74.877	26.115	1.00	32.13	B
ATOM	3064	O	GLY	B	85	75.961	74.257	25.200	1.00	25.66	B
ATOM	3065	N	SER	B	86	75.094	74.293	27.281	1.00	24.97	B
ATOM	3066	CA	SER	B	86	75.347	72.859	27.473	1.00	34.32	B
ATOM	3067	CB	SER	B	86	76.755	72.588	28.034	1.00	31.54	B
ATOM	3068	OG	SER	B	86	76.964	73.322	29.223	1.00	42.05	B
ATOM	3069	C	SER	B	86	74.315	72.304	28.415	1.00	27.65	B
ATOM	3070	O	SER	B	86	73.536	73.064	28.979	1.00	24.75	B
ATOM	3071	N	THR	B	87	74.294	70.982	28.573	1.00	27.03	B
ATOM	3072	CA	THR	B	87	73.325	70.314	29.454	1.00	29.87	B
ATOM	3073	CB	THR	B	87	73.532	68.806	29.450	1.00	34.20	B
ATOM	3074	OG1	THR	B	87	73.876	68.395	28.125	1.00	54.47	B
ATOM	3075	CG2	THR	B	87	72.263	68.107	29.856	1.00	36.26	B
ATOM	3076	C	THR	B	87	73.420	70.767	30.903	1.00	30.09	B
ATOM	3077	O	THR	B	87	74.501	71.113	31.381	1.00	30.94	B
ATOM	3078	N	PRO	B	88	72.293	70.771	31.626	1.00	26.03	B

ATOM	3079	CD	PRO	B	88	72.370	71.088	33.060	1.00	30.64	B
ATOM	3080	CA	PRO	B	88	70.921	70.406	31.240	1.00	33.13	B
ATOM	3081	CB	PRO	B	88	70.225	70.211	32.585	1.00	28.86	B
ATOM	3082	CG	PRO	B	88	70.903	71.248	33.440	1.00	31.91	B
ATOM	3083	C	PRO	B	88	70.228	71.482	30.338	1.00	31.83	B
ATOM	3084	O	PRO	B	88	70.495	72.668	30.535	1.00	29.33	B
ATOM	3085	N	TYR	B	89	69.340	71.059	29.503	1.00	27.84	B
ATOM	3086	CA	TYR	B	89	68.613	71.990	28.641	1.00	29.55	B
ATOM	3087	CB	TYR	B	89	68.553	71.414	27.239	1.00	27.73	B
ATOM	3088	CG	TYR	B	89	69.938	71.078	26.722	1.00	29.87	B
ATOM	3089	CD1	TYR	B	89	70.326	69.759	26.501	1.00	33.12	B
ATOM	3090	CE1	TYR	B	89	71.605	69.456	26.036	1.00	26.70	B
ATOM	3091	CD2	TYR	B	89	70.865	72.086	25.467	1.00	32.19	B
ATOM	3092	CE2	TYR	B	89	72.134	71.795	26.007	1.00	28.60	B
ATOM	3093	CZ	TYR	B	89	72.492	70.482	25.802	1.00	27.81	B
ATOM	3094	OH	TYR	B	89	73.770	70.211	25.415	1.00	32.86	B
ATOM	3095	C	TYR	B	89	67.212	72.242	29.176	1.00	25.88	B
ATOM	3096	O	TYR	B	89	66.333	71.400	29.025	1.00	25.96	B
ATOM	3097	N	ARG	B	90	67.015	73.405	29.790	1.00	25.05	B
ATOM	3098	CA	ARG	B	90	65.732	73.778	30.386	1.00	21.94	B
ATOM	3099	CB	ARG	B	90	65.950	74.306	31.802	1.00	25.43	B
ATOM	3100	CG	ARG	B	90	66.836	73.368	32.650	1.00	35.30	B
ATOM	3101	CD	ARG	B	90	66.308	71.933	32.684	1.00	30.92	B
ATOM	3102	NE	ARG	B	90	65.162	71.857	33.578	1.00	38.77	B
ATOM	3103	CZ	ARG	B	90	64.577	70.721	33.950	1.00	43.50	B
ATOM	3104	NH1	ARG	B	90	65.038	69.562	33.500	1.00	42.19	B
ATOM	3105	NH2	ARG	B	90	63.529	70.750	34.771	1.00	39.16	B
ATOM	3106	C	ARG	B	90	65.001	74.823	29.580	1.00	26.84	B
ATOM	3107	O	ARG	B	90	65.540	75.372	28.606	1.00	21.63	B
ATOM	3108	N	HIS	B	91	63.767	75.095	29.999	1.00	24.57	B
ATOM	3109	CA	HIS	B	91	62.903	76.057	29.318	1.00	28.69	B
ATOM	3110	CB	HIS	B	91	61.570	76.143	30.062	1.00	26.54	B
ATOM	3111	CG	HIS	B	91	60.516	76.909	29.326	1.00	34.66	B
ATOM	3112	CD2	HIS	B	91	59.414	77.563	29.770	1.00	26.97	B
ATOM	3113	ND1	HIS	B	91	60.513	77.035	27.952	1.00	29.34	B
ATOM	3114	CE1	HIS	B	91	59.457	77.735	27.582	1.00	27.63	B
ATOM	3115	NE2	HIS	B	91	58.775	78.066	28.666	1.00	34.45	B
ATOM	3116	C	HIS	B	91	63.546	77.445	29.177	1.00	30.22	B
ATOM	3117	O	HIS	B	91	63.937	78.069	30.161	1.00	23.98	B
ATOM	3118	N	GLY	B	92	63.663	77.915	27.941	1.00	26.25	B
ATOM	3119	CA	GLY	B	92	64.260	79.209	27.702	1.00	20.48	B
ATOM	3120	C	GLY	B	92	65.752	79.118	27.458	1.00	24.40	B
ATOM	3121	O	GLY	B	92	66.310	80.100	27.019	1.00	24.34	B
ATOM	3122	N	ASP	B	93	66.407	77.974	27.724	1.00	20.35	B
ATOM	3123	CA	ASP	B	93	67.857	77.884	27.472	1.00	19.73	B
ATOM	3124	CB	ASP	B	93	68.487	76.575	27.902	1.00	23.61	B
ATOM	3125	CG	ASP	B	93	68.579	76.504	29.504	1.00	20.60	B
ATOM	3126	OD1	ASP	B	93	68.336	77.522	30.167	1.00	23.89	B
ATOM	3127	OD2	ASP	B	93	68.884	75.401	30.020	1.00	25.06	B
ATOM	3128	C	ASP	B	93	68.138	77.911	25.981	1.00	25.02	B
ATOM	3129	O	ASP	B	93	67.362	77.415	25.170	1.00	24.06	B
ATOM	3130	N	SER	B	94	69.298	78.422	25.625	1.00	21.77	B
ATOM	3131	CA	SER	B	94	69.641	78.511	24.229	1.00	27.05	B
ATOM	3132	CB	SER	B	94	69.779	79.972	23.834	1.00	28.57	B
ATOM	3133	OG	SER	B	94	70.417	80.035	22.587	1.00	38.84	B

ATOM	3134	C	SER	B	94	70.935	77.815	23.908	1.00	25.71	B
ATOM	3135	O	SER	B	94	71.833	77.727	24.753	1.00	26.52	B
ATOM	3136	N	VAL	B	95	71.051	77.331	22.678	1.00	27.36	B
ATOM	3137	CA	VAL	B	95	72.291	76.689	22.245	1.00	26.56	B
ATOM	3138	CB	VAL	B	95	72.096	75.178	22.088	1.00	26.82	B
ATOM	3139	CG1	VAL	B	95	73.282	74.581	21.344	1.00	34.06	B
ATOM	3140	CG2	VAL	B	95	71.908	74.549	23.460	1.00	30.69	B
ATOM	3141	C	VAL	B	95	72.729	77.273	20.908	1.00	30.07	B
ATOM	3142	O	VAL	B	95	71.903	77.496	20.019	1.00	26.03	B
ATOM	3143	N	THR	B	96	74.026	77.526	20.758	1.00	27.23	B
ATOM	3144	CA	THR	B	96	74.540	78.058	19.503	1.00	23.14	B
ATOM	3145	CB	THR	B	96	75.242	79.419	19.687	1.00	32.77	B
ATOM	3146	OG1	THR	B	96	74.292	80.383	20.163	1.00	26.94	B
ATOM	3147	CG2	THR	B	96	75.845	79.896	18.329	1.00	26.13	B
ATOM	3148	C	THR	B	96	75.550	77.071	18.915	1.00	33.62	B
ATOM	3149	O	THR	B	96	76.445	76.614	19.618	1.00	26.19	B
ATOM	3150	N	PHE	B	97	75.381	76.732	17.638	1.00	28.29	B
ATOM	3151	CA	PHE	B	97	76.249	75.788	16.922	1.00	27.82	B
ATOM	3152	CB	PHE	B	97	75.409	74.849	16.039	1.00	27.23	B
ATOM	3153	CG	PHE	B	97	74.598	73.858	16.796	1.00	30.99	B
ATOM	3154	CD1	PHE	B	97	73.325	74.183	17.257	1.00	28.10	B
ATOM	3155	CD2	PHE	B	97	75.149	72.633	17.153	1.00	24.15	B
ATOM	3156	CE1	PHE	B	97	72.608	73.310	18.081	1.00	29.54	B
ATOM	3157	CE2	PHE	B	97	74.434	71.756	17.975	1.00	26.96	B
ATOM	3158	CZ	PHE	B	97	73.155	72.101	18.444	1.00	28.76	B
ATOM	3159	C	PHE	B	97	77.247	76.479	15.980	1.00	33.87	B
ATOM	3160	O	PHE	B	97	77.088	77.663	15.628	1.00	30.90	B
ATOM	3161	N	ALA	B	98	78.274	75.725	15.582	1.00	33.98	B
ATOM	3162	CA	ALA	B	98	79.266	76.152	14.574	1.00	34.14	B
ATOM	3163	CB	ALA	B	98	80.551	76.651	15.211	1.00	38.55	B
ATOM	3164	C	ALA	B	98	79.544	74.880	13.785	1.00	36.15	B
ATOM	3165	O	ALA	B	98	79.370	73.775	14.312	1.00	35.98	B
ATOM	3166	N	CYS	B	99	79.953	75.018	12.527	1.00	38.50	B
ATOM	3167	CA	CYS	B	99	80.266	73.843	11.711	1.00	39.15	B
ATOM	3168	C	CYS	B	99	81.747	73.512	11.779	1.00	36.00	B
ATOM	3169	O	CYS	B	99	82.573	74.408	11.865	1.00	32.17	B
ATOM	3170	CB	CYS	B	99	79.901	74.086	10.251	1.00	42.12	B
ATOM	3171	SG	CYS	B	99	78.108	74.162	9.949	1.00	40.52	B
ATOM	3172	N	LYS	B	100	82.089	72.229	11.749	1.00	35.70	B
ATOM	3173	CA	LYS	B	100	83.498	71.842	11.770	1.00	40.35	B
ATOM	3174	CB	LYS	B	100	83.632	70.319	11.848	1.00	43.13	B
ATOM	3175	CG	LYS	B	100	83.185	69.707	13.148	1.00	38.59	B
ATOM	3176	CD	LYS	B	100	82.771	68.263	12.966	1.00	44.87	B
ATOM	3177	CE	LYS	B	100	82.689	67.562	14.314	1.00	48.06	B
ATOM	3178	NZ	LYS	B	100	82.353	66.122	14.196	1.00	53.59	B
ATOM	3179	C	LYS	B	100	84.190	72.329	10.482	1.00	45.56	B
ATOM	3180	O	LYS	B	100	83.532	72.770	9.525	1.00	42.57	B
ATOM	3181	N	THR	B	101	85.519	72.239	10.456	1.00	47.30	B
ATOM	3182	CA	THR	B	101	86.286	72.651	9.282	1.00	48.55	B
ATOM	3183	CB	THR	B	101	87.794	72.408	9.497	1.00	48.03	B
ATOM	3184	OG1	THR	B	101	88.281	73.285	10.521	1.00	47.14	B
ATOM	3185	CG2	THR	B	101	88.557	72.683	8.212	1.00	51.80	B
ATOM	3186	C	THR	B	101	85.816	71.876	8.042	1.00	47.72	B
ATOM	3187	O	THR	B	101	85.523	70.681	8.127	1.00	43.56	B
ATOM	3188	N	ASN	B	102	85.747	72.555	6.901	1.00	47.11	B

ATOM	3189	CA	ASN	B	102	85.294	71.943	5.647	1.00 48.36	B
ATOM	3190	CB	ASN	B	102	85.961	70.594	5.375	1.00 53.67	B
ATOM	3191	CG	ASN	B	102	87.461	70.703	5.219	1.00 58.65	B
ATOM	3192	OD1	ASN	B	102	87.980	71.763	4.856	1.00 59.24	B
ATOM	3193	ND2	ASN	B	102	88.171	69.599	5.484	1.00 61.19	B
ATOM	3194	C	ASN	B	102	83.797	71.728	5.632	1.00 49.36	B
ATOM	3195	O	ASN	B	102	83.284	70.965	4.814	1.00 51.85	B
ATOM	3196	N	PHE	B	103	83.097	72.378	6.555	1.00 48.85	B
ATOM	3197	CA	PHE	B	103	81.641	72.294	6.617	1.00 44.54	B
ATOM	3198	CB	PHE	B	103	81.179	71.539	7.855	1.00 44.01	B
ATOM	3199	CG	PHE	B	103	81.335	70.067	7.740	1.00 45.42	B
ATOM	3200	CD1	PHE	B	103	82.554	69.461	8.037	1.00 47.36	B
ATOM	3201	CD2	PHE	B	103	80.270	69.274	7.323	1.00 44.68	B
ATOM	3202	CE1	PHE	B	103	82.715	68.064	7.921	1.00 44.91	B
ATOM	3203	CE2	PHE	B	103	80.413	67.883	7.202	1.00 46.13	B
ATOM	3204	CZ	PHE	B	103	81.638	67.276	7.503	1.00 44.51	B
ATOM	3205	C	PHE	B	103	81.103	73.700	6.663	1.00 43.79	B
ATOM	3206	O	PHE	B	103	81.736	74.577	7.239	1.00 41.42	B
ATOM	3207	N	SER	B	104	79.939	73.908	6.052	1.00 46.45	B
ATOM	3208	CA	SER	B	104	79.306	75.216	6.007	1.00 47.47	B
ATOM	3209	CB	SER	B	104	79.176	75.706	4.570	1.00 53.61	B
ATOM	3210	OG	SER	B	104	77.886	75.379	4.057	1.00 61.85	B
ATOM	3211	C	SER	B	104	77.921	75.051	6.596	1.00 46.27	B
ATOM	3212	O	SER	B	104	77.285	74.007	6.425	1.00 46.36	B
ATOM	3213	N	MET	B	105	77.435	76.089	7.269	1.00 47.80	B
ATOM	3214	CA	MET	B	105	76.129	75.998	7.913	1.00 50.16	B
ATOM	3215	CB	MET	B	105	76.114	76.848	9.184	1.00 42.24	B
ATOM	3216	CG	MET	B	105	74.783	76.829	9.931	1.00 39.50	B
ATOM	3217	SD	MET	B	105	74.951	77.585	11.559	1.00 31.98	B
ATOM	3218	CE	MET	B	105	76.153	76.456	12.300	1.00 32.14	B
ATOM	3219	C	MET	B	105	74.948	76.398	7.046	1.00 52.75	B
ATOM	3220	O	MET	B	105	75.066	77.234	6.147	1.00 52.67	B
ATOM	3221	N	ASN	B	106	73.807	75.787	7.343	1.00 57.19	B
ATOM	3222	CA	ASN	B	106	72.560	76.072	6.664	1.00 56.25	B
ATOM	3223	CB	ASN	B	106	72.186	74.950	5.722	1.00 63.78	B
ATOM	3224	CG	ASN	B	106	72.678	75.210	4.332	1.00 72.25	B
ATOM	3225	OD1	ASN	B	106	72.787	76.372	3.916	1.00 78.63	B
ATOM	3226	ND2	ASN	B	106	72.995	74.141	3.597	1.00 74.20	B
ATOM	3227	C	ASN	B	106	71.504	76.200	7.727	1.00 54.17	B
ATOM	3228	O	ASN	B	106	71.303	75.277	8.508	1.00 56.24	B
ATOM	3229	N	GLY	B	107	70.833	77.342	7.762	1.00 50.67	B
ATOM	3230	CA	GLY	B	107	69.805	77.552	8.763	1.00 44.02	B
ATOM	3231	C	GLY	B	107	70.334	78.414	9.886	1.00 42.66	B
ATOM	3232	O	GLY	B	107	71.478	78.864	9.854	1.00 41.68	B
ATOM	3233	N	ASN	B	108	69.500	78.646	10.889	1.00 46.24	B
ATOM	3234	CA	ASN	B	108	69.878	79.464	12.032	1.00 47.08	B
ATOM	3235	CB	ASN	B	108	68.613	79.910	12.751	1.00 55.45	B
ATOM	3236	CG	ASN	B	108	67.793	80.852	11.903	1.00 63.30	B
ATOM	3237	OD1	ASN	B	108	68.164	82.013	11.722	1.00 67.44	B
ATOM	3238	ND2	ASN	B	108	66.691	80.352	11.346	1.00 68.11	B
ATOM	3239	C	ASN	B	108	70.808	78.723	12.981	1.00 39.04	B
ATOM	3240	O	ASN	B	108	70.560	77.577	13.347	1.00 33.47	B
ATOM	3241	N	LYS	B	109	71.858	79.406	13.402	1.00 34.53	B
ATOM	3242	CA	LYS	B	109	72.859	78.806	14.280	1.00 35.55	B
ATOM	3243	CB	LYS	B	109	74.138	79.632	14.217	1.00 35.53	B

ATOM	3244	CG	LYS	B	109	73.909	81.037	14.698	1.00	37.21	B
ATOM	3245	CD	LYS	B	109	75.176	81.691	15.171	1.00	43.67	B
ATOM	3246	CE	LYS	B	109	74.913	83.141	15.501	1.00	53.84	B
ATOM	3247	NZ	LYS	B	109	76.079	83.848	16.124	1.00	67.33	B
ATOM	3248	C	LYS	B	109	72.456	78.639	15.753	1.00	33.59	B
ATOM	3249	O	LYS	B	109	73.116	77.900	16.490	1.00	32.99	B
ATOM	3250	N	SER	B	110	71.409	79.337	16.198	1.00	29.02	B
ATOM	3251	CA	SER	B	110	70.972	79.239	17.597	1.00	31.62	B
ATOM	3252	CB	SER	B	110	71.068	80.588	18.298	1.00	28.39	B
ATOM	3253	OG	SER	B	110	72.395	81.073	18.276	1.00	35.28	B
ATOM	3254	C	SER	B	110	69.547	78.730	17.734	1.00	33.04	B
ATOM	3255	O	SER	B	110	68.665	79.049	16.935	1.00	28.18	B
ATOM	3256	N	VAL	B	111	69.336	77.927	18.761	1.00	32.94	B
ATOM	3257	CA	VAL	B	111	68.028	77.360	19.032	1.00	28.12	B
ATOM	3258	CB	VAL	B	111	67.998	75.911	18.507	1.00	34.53	B
ATOM	3259	CG1	VAL	B	111	69.117	75.074	19.143	1.00	27.59	B
ATOM	3260	CG2	VAL	B	111	66.694	75.304	18.785	1.00	41.47	B
ATOM	3261	C	VAL	B	111	67.729	77.488	20.539	1.00	26.65	B
ATOM	3262	O	VAL	B	111	68.631	77.621	21.359	1.00	27.71	B
ATOM	3263	N	TRP	B	112	66.447	77.496	20.866	1.00	26.33	B
ATOM	3264	CA	TRP	B	112	65.932	77.654	22.205	1.00	21.46	B
ATOM	3265	CB	TRP	B	112	65.023	78.895	22.287	1.00	27.43	B
ATOM	3266	CG	TRP	B	112	65.772	80.142	22.392	1.00	28.72	B
ATOM	3267	CD2	TRP	B	112	66.455	80.818	21.323	1.00	27.13	B
ATOM	3268	CE2	TRP	B	112	67.130	81.922	21.894	1.00	23.65	B
ATOM	3269	CE3	TRP	B	112	66.560	80.595	19.944	1.00	27.06	B
ATOM	3270	CD1	TRP	B	112	66.053	80.849	23.542	1.00	29.24	B
ATOM	3271	NE1	TRP	B	112	66.875	81.916	23.242	1.00	22.18	B
ATOM	3272	CZ2	TRP	B	112	67.896	82.804	21.132	1.00	24.55	B
ATOM	3273	CZ3	TRP	B	112	67.328	81.476	19.179	1.00	32.51	B
ATOM	3274	CH2	TRP	B	112	67.985	82.570	19.782	1.00	28.74	B
ATOM	3275	C	TRP	B	112	65.113	76.462	22.622	1.00	24.09	B
ATOM	3276	O	TRP	B	112	64.348	75.924	21.826	1.00	23.03	B
ATOM	3277	N	CYS	B	113	65.257	76.065	23.886	1.00	16.00	B
ATOM	3278	CA	CYS	B	113	64.507	74.942	24.421	1.00	22.66	B
ATOM	3279	C	CYS	B	113	63.090	75.442	24.775	1.00	27.37	B
ATOM	3280	O	CYS	B	113	62.892	76.248	25.702	1.00	23.71	B
ATOM	3281	CB	CYS	B	113	65.230	74.386	25.636	1.00	24.38	B
ATOM	3282	SG	CYS	B	113	64.295	73.084	26.474	1.00	25.70	B
ATOM	3283	N	GLN	B	114	62.105	74.973	24.014	1.00	22.77	B
ATOM	3284	CA	GLN	B	114	60.704	75.406	24.190	1.00	27.53	B
ATOM	3285	CB	GLN	B	114	59.993	75.312	22.852	1.00	23.87	B
ATOM	3286	CG	GLN	B	114	60.669	76.101	21.776	1.00	25.80	B
ATOM	3287	CD	GLN	B	114	59.934	75.957	20.455	1.00	34.33	B
ATOM	3288	OE1	GLN	B	114	59.540	74.850	20.084	1.00	40.82	B
ATOM	3289	NE2	GLN	B	114	59.749	77.062	19.744	1.00	28.51	B
ATOM	3290	C	GLN	B	114	59.918	74.632	25.242	1.00	24.17	B
ATOM	3291	O	GLN	B	114	60.324	73.557	25.638	1.00	24.70	B
ATOM	3292	N	ALA	B	115	58.806	75.187	25.704	1.00	28.17	B
ATOM	3293	CA	ALA	B	115	57.984	74.520	26.720	1.00	32.79	B
ATOM	3294	CB	ALA	B	115	56.769	75.392	27.068	1.00	30.00	B
ATOM	3295	C	ALA	B	115	57.523	73.207	26.316	1.00	34.03	B
ATOM	3296	O	ALA	B	115	57.338	72.237	27.170	1.00	33.21	B
ATOM	3297	N	ASN	B	116	57.343	72.881	25.020	1.00	36.70	B
ATOM	3298	CA	ASN	B	116	56.913	71.573	24.526	1.00	38.02	B

ATOM	3299	CB	ASN	B	116	56.230	71.723	23.168	1.00	34.90	B
ATOM	3300	CG	ASN	B	116	57.198	72.144	22.087	1.00	33.42	B
ATOM	3301	OD1	ASN	B	116	58.359	72.454	22.364	1.00	28.93	B
ATOM	3302	ND2	ASN	B	116	56.728	72.147	20.853	1.00	30.98	B
ATOM	3303	C	ASN	B	116	58.104	70.608	24.392	1.00	34.77	B
ATOM	3304	O	ASN	B	116	58.017	69.610	23.695	1.00	37.59	B
ATOM	3305	N	ASN	B	117	59.219	70.997	25.044	1.00	36.92	B
ATOM	3306	CA	ASN	B	117	60.425	70.094	25.072	1.00	31.01	B
ATOM	3307	CB	ASN	B	117	60.095	68.758	25.699	1.00	35.95	B
ATOM	3308	CG	ASN	B	117	59.327	68.855	27.022	1.00	41.69	B
ATOM	3309	OD1	ASN	B	117	58.165	68.448	27.116	1.00	48.82	B
ATOM	3310	ND2	ASN	B	117	59.966	69.423	28.041	1.00	38.48	B
ATOM	3311	C	ASN	B	117	61.155	69.913	23.753	1.00	35.04	B
ATOM	3312	O	ASN	B	117	61.989	69.010	23.584	1.00	30.97	B
ATOM	3313	N	MET	B	118	60.877	71.804	22.814	1.00	32.90	B
ATOM	3314	CA	MET	B	118	61.544	70.747	21.539	1.00	30.69	B
ATOM	3315	CB	MET	B	118	60.533	70.486	20.426	1.00	39.19	B
ATOM	3316	CG	MET	B	118	60.143	69.004	20.284	1.00	45.35	B
ATOM	3317	SD	MET	B	118	58.844	68.904	19.065	1.00	61.98	B
ATOM	3318	CE	MET	B	118	57.379	68.930	20.152	1.00	59.12	B
ATOM	3319	C	MET	B	118	62.299	72.033	21.290	1.00	32.74	B
ATOM	3320	O	MET	B	118	61.958	73.093	21.820	1.00	31.41	B
ATOM	3321	N	TRP	B	119	63.322	71.913	20.460	1.00	30.27	B
ATOM	3322	CA	TRP	B	119	64.197	73.097	20.122	1.00	32.04	B
ATOM	3323	CB	TRP	B	119	65.519	72.477	19.556	1.00	29.45	B
ATOM	3324	CG	TRP	B	119	66.377	71.888	20.618	1.00	34.08	B
ATOM	3325	CD2	TRP	B	119	67.091	72.613	21.638	1.00	29.55	B
ATOM	3326	CE2	TRP	B	119	67.641	71.653	22.514	1.00	32.16	B
ATOM	3327	CE3	TRP	B	119	67.309	73.974	21.891	1.00	27.61	B
ATOM	3328	CD1	TRP	B	119	66.533	70.563	20.907	1.00	27.66	B
ATOM	3329	NE1	TRP	B	119	67.287	70.419	22.045	1.00	29.97	B
ATOM	3330	CZ2	TRP	B	119	68.401	72.018	23.634	1.00	33.69	B
ATOM	3331	CZ3	TRP	B	119	68.067	74.353	23.002	1.00	28.67	B
ATOM	3332	CH2	TRP	B	119	68.603	73.356	23.860	1.00	29.17	B
ATOM	3333	C	TRP	B	119	63.672	74.059	19.188	1.00	35.37	B
ATOM	3334	O	TRP	B	119	62.946	73.750	18.264	1.00	34.01	B
ATOM	3335	N	GLY	B	120	64.129	75.279	19.507	1.00	44.82	B
ATOM	3336	CA	GLY	B	120	63.928	76.577	18.868	1.00	40.39	B
ATOM	3337	C	GLY	B	120	62.736	76.818	18.037	1.00	45.27	B
ATOM	3338	O	GLY	B	120	61.922	75.920	17.884	1.00	54.52	B
ATOM	3339	N	PRO	B	121	62.570	78.049	17.525	1.00	39.72	B
ATOM	3340	CD	PRO	B	121	63.331	79.268	17.805	1.00	34.64	B
ATOM	3341	CA	PRO	B	121	61.411	78.339	16.678	1.00	40.69	B
ATOM	3342	CB	PRO	B	121	61.355	79.869	16.674	1.00	33.54	B
ATOM	3343	CG	PRO	B	121	62.781	80.221	16.775	1.00	38.11	B
ATOM	3344	C	PRO	B	121	61.717	77.733	15.294	1.00	38.17	B
ATOM	3345	O	PRO	B	121	60.817	77.553	14.591	1.00	40.16	B
ATOM	3346	N	THR	B	122	62.994	77.693	14.930	1.00	33.84	B
ATOM	3347	CA	THR	B	122	63.424	77.113	13.660	1.00	38.91	B
ATOM	3348	CB	THR	B	122	64.548	77.939	12.988	1.00	42.26	B
ATOM	3349	OG1	THR	B	122	65.803	77.671	13.634	1.00	39.47	B
ATOM	3350	CG2	THR	B	122	64.259	79.431	13.106	1.00	40.58	B
ATOM	3351	C	THR	B	122	63.968	75.708	13.874	1.00	40.61	B
ATOM	3352	O	THR	B	122	64.163	75.266	14.999	1.00	43.52	B
ATOM	3353	N	ARG	B	123	64.220	75.005	12.784	1.00	42.70	B

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ATOM   3354  CA  ARG B 123      64.762  73.656  12.870  1.00 46.43      B
ATOM   3355  CB  ARG B 123      64.505  72.912  11.549  1.00 48.19      B
ATOM   3356  CG  ARG B 123      64.849  71.433  11.600  1.00 63.34      B
ATOM   3357  CD  ARG B 123      64.109  70.638  10.517  1.00 71.72      B
ATOM   3358  NE  ARG B 123      62.664  70.564  10.762  1.00 75.72      B
ATOM   3359  CZ  ARG B 123      61.734  70.934   9.881  1.00 77.53      B
ATOM   3360  NH1 ARG B 123      62.096  71.410   8.690  1.00 78.13      B
ATOM   3361  NH2 ARG B 123      60.444  70.820  10.184  1.00 75.29      B
ATOM   3362  C   ARG B 123      66.270  73.774  13.141  1.00 36.14      B
ATOM   3363  O   ARG B 123      66.861  74.816  12.880  1.00 34.06      B
ATOM   3364  N   LEU B 124      66.888  72.714  13.659  1.00 36.62      B
ATOM   3365  CA  LEU B 124      68.326  72.743  13.939  1.00 35.68      B
ATOM   3366  CB  LEU B 124      68.818  71.410  14.509  1.00 37.22      B
ATOM   3367  CG  LEU B 124      68.399  71.019  15.933  1.00 38.68      B
ATOM   3368  CD1 LEU B 124      69.008  69.670  16.342  1.00 37.12      B
ATOM   3369  CD2 LEU B 124      68.860  72.097  16.874  1.00 34.15      B
ATOM   3370  C   LEU B 124      69.081  73.029  12.656  1.00 37.07      B
ATOM   3371  O   LEU B 124      68.701  72.584  11.583  1.00 35.87      B
ATOM   3372  N   PRO B 125      70.168  73.787  12.750  1.00 40.36      B
ATOM   3373  CD  PRO B 125      70.832  74.306  13.962  1.00 38.05      B
ATOM   3374  CA  PRO B 125      70.933  74.085  11.538  1.00 35.47      B
ATOM   3375  CB  PRO B 125      71.993  75.069  12.029  1.00 35.51      B
ATOM   3376  CG  PRO B 125      72.224  74.641  13.460  1.00 35.57      B
ATOM   3377  C   PRO B 125      71.535  72.794  11.002  1.00 40.45      B
ATOM   3378  O   PRO B 125      71.432  71.739  11.640  1.00 33.92      B
ATOM   3379  N   THR B 126      72.131  72.867   9.814  1.00 41.58      B
ATOM   3380  CA  THR B 126      72.765  71.704   9.217  1.00 41.03      B
ATOM   3381  CB  THR B 126      71.929  71.137   8.006  1.00 42.99      B
ATOM   3382  OG1 THR B 126      71.625  72.182   7.075  1.00 45.10      B
ATOM   3383  CG2 THR B 126      70.628  70.529   8.503  1.00 40.83      B
ATOM   3384  C   THR B 126      74.157  72.116   8.777  1.00 41.16      B
ATOM   3385  O   THR B 126      74.415  73.299   8.544  1.00 40.35      B
ATOM   3386  N   CYS B 127      75.074  71.158   8.716  1.00 42.86      B
ATOM   3387  CA  CYS B 127      76.433  71.468   8.279  1.00 48.44      B
ATOM   3388  C   CYS B 127      76.774  70.561   7.098  1.00 53.76      B
ATOM   3389  O   CYS B 127      76.711  69.336   7.219  1.00 55.59      B
ATOM   3390  CB  CYS B 127      77.440  71.249   9.422  1.00 49.29      B
ATOM   3391  SG  CYS B 127      77.365  72.471  10.779  1.00 41.21      B
ATOM   3392  N   VAL B 128      77.117  71.159   5.960  1.00 52.99      B
ATOM   3393  CA  VAL B 128      77.466  70.386   4.764  1.00 58.11      B
ATOM   3394  CB  VAL B 128      76.479  70.674   3.612  1.00 60.17      B
ATOM   3395  CG1 VAL B 128      76.356  72.179   3.395  1.00 59.61      B
ATOM   3396  CG2 VAL B 128      76.974  70.005   2.322  1.00 62.78      B
ATOM   3397  C   VAL B 128      78.881  70.738   4.290  1.00 55.96      B
ATOM   3398  O   VAL B 128      79.307  71.875   4.427  1.00 56.76      B
ATOM   3399  N   SER B 129      79.604  69.763   3.747  1.00 58.88      B
ATOM   3400  CA  SER B 129      80.976  69.974   3.241  1.00 63.04      B
ATOM   3401  CB  SER B 129      81.489  68.685   2.616  1.00 64.42      B
ATOM   3402  OG  SER B 129      80.566  68.240   1.633  1.00 74.77      B
ATOM   3403  C   SER B 129      81.061  71.092   2.194  1.00 60.01      B
ATOM   3404  O   SER B 129      82.054  71.856   2.166  1.00 59.63      B
ATOM   3405  OXT SER B 129      80.121  71.165   1.381  1.00 61.43      B
END
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TABLE 3

	ATOM	2419	CB	ALA	B	1	64.181	107.666	4.123	1.00	39.20	B
	ATOM	2420	C	ALA	B	1	62.836	105.816	3.113	1.00	41.03	B
	ATOM	2421	O	ALA	B	1	61.659	105.713	3.477	1.00	42.08	B
	ATOM	2422	N	ALA	B	1	62.413	108.231	2.458	1.00	40.18	B
	ATOM	2423	CA	ALA	B	1	63.447	107.201	2.861	1.00	43.96	B
	ATOM	2424	N	ILE	B	2	63.636	104.759	2.923	1.00	39.63	B
	ATOM	2425	CA	ILE	B	2	63.175	103.383	3.141	1.00	37.01	B
	ATOM	2426	CB	ILE	B	2	64.245	102.349	2.700	1.00	32.57	B
	ATOM	2427	CG2	ILE	B	2	63.775	100.936	3.064	1.00	35.80	B
	ATOM	2428	CG1	ILE	B	2	64.457	102.422	1.178	1.00	34.01	B
	ATOM	2429	CD1	ILE	B	2	65.479	101.372	0.650	1.00	31.21	B
	ATOM	2430	C	ILE	B	2	62.831	103.151	4.633	1.00	38.27	B
	ATOM	2431	O	ILE	B	2	63.565	103.577	5.528	1.00	32.71	B
	ATOM	2432	N	SER	B	3	61.714	102.486	4.897	1.00	30.65	B
	ATOM	2433	CA	SER	B	3	61.316	102.226	6.272	1.00	26.19	B
	ATOM	2434	CB	SER	B	3	60.245	103.236	6.689	1.00	31.79	B
	ATOM	2435	OG	SER	B	3	59.060	103.020	5.926	1.00	27.35	B
	ATOM	2436	C	SER	B	3	60.744	100.826	6.435	1.00	30.38	B
	ATOM	2437	O	SER	B	3	60.495	100.132	5.446	1.00	28.89	B
	ATOM	2438	N	CYS	B	4	60.559	100.410	7.690	1.00	27.89	B
	ATOM	2439	CA	CYS	B	4	59.941	99.127	8.003	1.00	27.29	B
	ATOM	2440	C	CYS	B	4	58.609	99.528	8.600	1.00	26.13	B
	ATOM	2441	O	CYS	B	4	58.446	100.666	9.061	1.00	29.64	B
	ATOM	2442	CB	CYS	B	4	60.731	98.328	9.056	1.00	27.46	B
	ATOM	2443	SG	CYS	B	4	62.214	97.531	8.369	1.00	27.76	B
	ATOM	2444	N	GLY	B	5	57.648	98.622	8.561	1.00	22.65	B
	ATOM	2445	CA	GLY	B	5	56.366	98.916	9.155	1.00	23.57	B
	ATOM	2446	C	GLY	B	5	56.452	98.570	10.643	1.00	24.00	B
	ATOM	2447	O	GLY	B	5	57.504	98.199	11.181	1.00	23.18	B
	ATOM	2448	N	SER	B	6	55.322	98.698	11.313	1.00	21.65	B
	ATOM	2449	CA	SER	B	6	55.204	98.441	12.733	1.00	22.23	B
	ATOM	2450	CB	SER	B	6	53.722	98.511	13.098	1.00	27.49	B
	ATOM	2451	OG	SER	B	6	53.543	98.605	14.483	1.00	33.82	B
	ATOM	2452	C	SER	B	6	55.785	97.062	13.091	1.00	26.45	B
	ATOM	2453	O	SER	B	6	55.489	96.081	12.439	1.00	22.14	B
	ATOM	2454	N	PRO	B	7	56.639	96.980	14.122	1.00	26.74	B
	ATOM	2455	CD	PRO	B	7	57.230	98.026	14.973	1.00	25.89	B
	ATOM	2456	CA	PRO	B	7	57.191	95.661	14.468	1.00	25.01	B
	ATOM	2457	CB	PRO	B	7	58.175	95.984	15.592	1.00	22.52	B
	ATOM	2458	CG	PRO	B	7	57.589	97.228	16.232	1.00	26.49	B
	ATOM	2459	C	PRO	B	7	56.133	94.627	14.894	1.00	27.04	B
	ATOM	2460	O	PRO	B	7	55.061	94.961	15.414	1.00	24.19	B
	ATOM	2461	N	PRO	B	8	56.439	93.345	14.700	1.00	24.37	B
	ATOM	2462	CD	PRO	B	8	57.540	92.754	13.936	1.00	20.75	B
	ATOM	2463	CA	PRO	B	8	55.431	92.366	15.099	1.00	25.28	B
	ATOM	2464	CB	PRO	B	8	55.974	91.048	14.538	1.00	31.15	B
	ATOM	2465	CG	PRO	B	8	57.401	91.314	14.245	1.00	33.33	B
	ATOM	2466	C	PRO	B	8	55.228	92.382	16.613	1.00	30.70	B
	ATOM	2467	O	PRO	B	8	56.180	92.527	17.364	1.00	31.22	B
	ATOM	2468	N	PRO	B	9	53.971	92.314	17.074	1.00	30.39	B
	ATOM	2469	CD	PRO	B	9	52.724	92.280	16.275	1.00	37.82	B
	ATOM	2470	CA	PRO	B	9	53.686	92.322	18.518	1.00	32.22	B
	ATOM	2471	CB	PRO	B	9	52.155	92.415	18.589	1.00	31.66	B

ATOM	2472	CG	PRO	B	9	51.705	91.731	17.265	1.00	31.37	B
ATOM	2473	C	PRO	B	9	54.190	91.062	19.209	1.00	26.54	B
ATOM	2474	O	PRO	B	9	54.542	90.072	18.563	1.00	23.13	B
ATOM	2475	N	ILE	B	10	54.214	91.111	20.526	1.00	25.96	B
ATOM	2476	CA	ILE	B	10	54.651	89.969	21.302	1.00	34.36	B
ATOM	2477	CB	ILE	B	10	56.150	90.068	21.770	1.00	24.92	B
ATOM	2478	CG2	ILE	B	10	56.398	91.363	22.562	1.00	24.04	B
ATOM	2479	CG1	ILE	B	10	56.491	88.795	22.581	1.00	30.43	B
ATOM	2480	CD1	ILE	B	10	57.991	88.536	22.813	1.00	24.83	B
ATOM	2481	C	ILE	B	10	53.753	89.810	22.511	1.00	33.31	B
ATOM	2482	O	ILE	B	10	53.743	90.647	23.412	1.00	32.83	B
ATOM	2483	N	LEU	B	11	52.992	88.724	22.525	1.00	30.71	B
ATOM	2484	CA	LEU	B	11	52.108	88.483	23.659	1.00	34.63	B
ATOM	2485	CB	LEU	B	11	51.217	87.277	23.365	1.00	36.50	B
ATOM	2486	CG	LEU	B	11	50.279	87.435	22.161	1.00	41.37	B
ATOM	2487	CD1	LEU	B	11	49.708	86.073	21.769	1.00	42.99	B
ATOM	2488	CD2	LEU	B	11	49.142	88.425	22.495	1.00	39.65	B
ATOM	2489	C	LEU	B	11	52.912	88.247	24.946	1.00	33.24	B
ATOM	2490	O	LEU	B	11	53.905	87.517	24.948	1.00	28.06	B
ATOM	2491	N	ASN	B	12	52.463	88.872	26.032	1.00	31.32	B
ATOM	2492	CA	ASN	B	12	53.086	88.753	27.328	1.00	30.29	B
ATOM	2493	CB	ASN	B	12	53.025	87.303	27.802	1.00	32.27	B
ATOM	2494	CG	ASN	B	12	51.612	86.875	28.083	1.00	38.86	B
ATOM	2495	OD1	ASN	B	12	50.917	87.526	28.864	1.00	38.59	B
ATOM	2496	ND2	ASN	B	12	51.161	85.805	27.431	1.00	34.66	B
ATOM	2497	C	ASN	B	12	54.510	89.250	27.371	1.00	32.36	B
ATOM	2498	O	ASN	B	12	55.277	88.858	28.239	1.00	32.56	B
ATOM	2499	N	GLY	B	13	54.849	90.130	26.439	1.00	28.46	B
ATOM	2500	CA	GLY	B	13	56.187	90.671	26.400	1.00	28.72	B
ATOM	2501	C	GLY	B	13	56.147	92.166	26.169	1.00	29.80	B
ATOM	2502	O	GLY	B	13	55.075	92.780	26.153	1.00	34.03	B
ATOM	2503	N	ARG	B	14	57.324	92.742	25.983	1.00	28.15	B
ATOM	2504	CA	ARG	B	14	57.486	94.166	25.739	1.00	31.15	B
ATOM	2505	CB	ARG	B	14	58.198	94.882	26.897	1.00	34.62	B
ATOM	2506	CG	ARG	B	14	57.388	95.196	28.116	1.00	41.11	B
ATOM	2507	CD	ARG	B	14	58.240	95.962	29.112	1.00	42.09	B
ATOM	2508	NE	ARG	B	14	57.526	96.080	30.373	1.00	49.55	B
ATOM	2509	CZ	ARG	B	14	58.023	96.595	31.487	1.00	48.40	B
ATOM	2510	NH1	ARG	B	14	59.261	97.065	31.509	1.00	40.72	B
ATOM	2511	NH2	ARG	B	14	57.276	96.602	32.593	1.00	56.30	B
ATOM	2512	C	ARG	B	14	58.409	94.342	24.567	1.00	23.56	B
ATOM	2513	O	ARG	B	14	59.232	93.480	24.280	1.00	23.51	B
ATOM	2514	N	ILE	B	15	58.319	95.516	23.955	1.00	27.48	B
ATOM	2515	CA	ILE	B	15	59.171	95.893	22.841	1.00	26.75	B
ATOM	2516	CB	ILE	B	15	58.345	96.176	21.580	1.00	26.32	B
ATOM	2517	CG2	ILE	B	15	59.250	96.815	20.497	1.00	29.30	B
ATOM	2518	CG1	ILE	B	15	57.656	94.902	21.122	1.00	30.62	B
ATOM	2519	CD1	ILE	B	15	56.760	95.100	19.889	1.00	35.21	B
ATOM	2520	C	ILE	B	15	59.767	97.212	23.279	1.00	26.59	B
ATOM	2521	O	ILE	B	15	59.050	98.050	23.818	1.00	30.94	B
ATOM	2522	N	SER	B	16	61.055	97.409	23.036	1.00	23.15	B
ATOM	2523	CA	SER	B	16	61.709	98.654	23.393	1.00	32.61	B
ATOM	2524	CB	SER	B	16	63.187	98.567	23.057	1.00	29.32	B
ATOM	2525	OG	SER	B	16	63.359	98.151	21.717	1.00	35.31	B
ATOM	2526	C	SER	B	16	61.082	99.839	22.639	1.00	41.27	B

ATOM	2527	O	SER	B	16	60.466	99.674	21.576	1.00	36.78	B
ATOM	2528	N	TYR	B	17	61.260	101.035	23.193	1.00	42.89	B
ATOM	2529	CA	TYR	B	17	60.719	102.267	22.624	1.00	46.29	B
ATOM	2530	CB	TYR	B	17	60.932	103.436	23.623	1.00	44.99	B
ATOM	2531	CG	TYR	B	17	60.026	103.380	24.865	1.00	47.02	B
ATOM	2532	CD1	TYR	B	17	60.510	103.694	26.151	1.00	49.03	B
ATOM	2533	CE1	TYR	B	17	59.664	103.655	27.283	1.00	48.52	B
ATOM	2534	CD2	TYR	B	17	58.686	103.025	24.748	1.00	51.67	B
ATOM	2535	CE2	TYR	B	17	57.833	102.974	25.861	1.00	53.32	B
ATOM	2536	CZ	TYR	B	17	58.319	103.292	27.122	1.00	56.82	B
ATOM	2537	OH	TYR	B	17	57.430	103.259	28.190	1.00	55.53	B
ATOM	2538	C	TYR	B	17	61.397	102.551	21.285	1.00	46.15	B
ATOM	2539	O	TYR	B	17	62.600	102.375	21.146	1.00	50.00	B
ATOM	2540	N	TYR	B	18	60.623	102.952	20.281	1.00	46.05	B
ATOM	2541	CA	TYR	B	18	61.204	103.270	18.975	1.00	44.93	B
ATOM	2542	CB	TYR	B	18	61.076	102.076	18.010	1.00	37.78	B
ATOM	2543	CG	TYR	B	18	59.645	101.669	17.711	1.00	37.10	B
ATOM	2544	CD1	TYR	B	18	58.890	102.343	16.750	1.00	31.24	B
ATOM	2545	CE1	TYR	B	18	57.573	101.980	16.501	1.00	34.43	B
ATOM	2546	CD2	TYR	B	18	59.040	100.622	18.415	1.00	34.57	B
ATOM	2547	CE2	TYR	B	18	57.730	100.255	18.184	1.00	36.06	B
ATOM	2548	CZ	TYR	B	18	57.000	100.939	17.218	1.00	35.02	B
ATOM	2549	OH	TYR	B	18	55.706	100.565	16.967	1.00	33.22	B
ATOM	2550	C	TYR	B	18	60.524	104.514	18.375	1.00	40.62	B
ATOM	2551	O	TYR	B	18	59.356	104.784	18.632	1.00	40.57	B
ATOM	2552	N	SER	B	19	61.280	105.260	17.586	1.00	42.39	B
ATOM	2553	CA	SER	B	19	60.786	106.464	16.931	1.00	49.17	B
ATOM	2554	CB	SER	B	19	61.922	107.472	16.789	1.00	49.59	B
ATOM	2555	OG	SER	B	19	63.070	106.843	16.237	1.00	54.17	B
ATOM	2556	C	SER	B	19	60.213	106.155	15.540	1.00	51.20	B
ATOM	2557	O	SER	B	19	60.569	105.165	14.900	1.00	42.62	B
ATOM	2558	N	THR	B	20	59.347	107.041	15.073	1.00	48.91	B
ATOM	2559	CA	THR	B	20	58.706	106.898	13.783	1.00	49.40	B
ATOM	2560	CB	THR	B	20	57.166	107.002	13.991	1.00	52.73	B
ATOM	2561	OG1	THR	B	20	56.483	106.279	12.968	1.00	60.25	B
ATOM	2562	CG2	THR	B	20	56.714	108.456	13.943	1.00	51.71	B
ATOM	2563	C	THR	B	20	59.222	108.022	12.844	1.00	47.48	B
ATOM	2564	O	THR	B	20	59.460	109.147	13.280	1.00	50.56	B
ATOM	2565	N	PRO	B	21	59.427	107.720	11.551	1.00	46.52	B
ATOM	2566	CD	PRO	B	21	59.801	108.745	10.551	1.00	44.33	B
ATOM	2567	CA	PRO	B	21	59.204	106.417	10.909	1.00	43.20	B
ATOM	2568	CB	PRO	B	21	59.137	106.769	9.422	1.00	43.49	B
ATOM	2569	CG	PRO	B	21	60.103	107.918	9.305	1.00	44.19	B
ATOM	2570	C	PRO	B	21	60.342	105.456	11.248	1.00	37.71	B
ATOM	2571	O	PRO	B	21	61.393	105.891	11.674	1.00	38.42	B
ATOM	2572	N	THR	B	22	60.123	104.155	11.067	1.00	40.00	B
ATOM	2573	CA	THR	B	22	61.139	103.150	11.382	1.00	37.29	B
ATOM	2574	CB	THR	B	22	60.521	101.715	11.578	1.00	33.63	B
ATOM	2575	OG1	THR	B	22	59.497	101.719	12.600	1.00	36.55	B
ATOM	2576	CG2	THR	B	22	61.626	100.734	11.963	1.00	26.59	B
ATOM	2577	C	THR	B	22	62.143	103.079	10.221	1.00	35.94	B
ATOM	2578	O	THR	B	22	61.851	102.484	9.183	1.00	33.29	B
ATOM	2579	N	ALA	B	23	63.326	103.663	10.410	1.00	33.77	B
ATOM	2580	CA	ALA	B	23	64.367	103.677	9.380	1.00	30.19	B
ATOM	2581	CB	ALA	B	23	65.314	104.852	9.615	1.00	28.90	B

ATOM	2582	C	ALA	B	23	65.192	102.399	9.300	1.00	30.98	B
ATOM	2583	O	ALA	B	23	65.331	101.693	10.284	1.00	23.97	B
ATOM	2584	N	VAL	B	24	65.736	102.127	8.112	1.00	27.61	B
ATOM	2585	CA	VAL	B	24	66.591	100.982	7.874	1.00	26.92	B
ATOM	2586	CB	VAL	B	24	67.147	101.042	6.460	1.00	29.41	B
ATOM	2587	CG1	VAL	B	24	68.357	100.043	6.326	1.00	28.58	B
ATOM	2588	CG2	VAL	B	24	66.107	100.729	5.430	1.00	26.92	B
ATOM	2589	C	VAL	B	24	67.707	101.091	8.898	1.00	32.79	B
ATOM	2590	O	VAL	B	24	68.266	102.166	9.077	1.00	26.10	B
ATOM	2591	N	GLY	B	25	68.036	100.000	9.586	1.00	28.01	B
ATOM	2592	CA	GLY	B	25	69.070	100.081	10.596	1.00	31.93	B
ATOM	2593	C	GLY	B	25	68.516	100.210	12.007	1.00	34.29	B
ATOM	2594	O	GLY	B	25	69.251	100.080	12.966	1.00	28.44	B
ATOM	2595	N	THR	B	26	67.227	100.486	12.148	1.00	26.99	B
ATOM	2596	CA	THR	B	26	66.650	100.568	13.474	1.00	29.37	B
ATOM	2597	CB	THR	B	26	65.179	100.994	13.403	1.00	30.78	B
ATOM	2598	OG1	THR	B	26	65.111	102.295	12.808	1.00	26.87	B
ATOM	2599	CG2	THR	B	26	64.524	101.000	14.833	1.00	23.56	B
ATOM	2600	C	THR	B	26	66.713	99.183	14.136	1.00	32.07	B
ATOM	2601	O	THR	B	26	66.462	98.171	13.473	1.00	28.44	B
ATOM	2602	N	VAL	B	27	67.056	99.143	15.429	1.00	28.90	B
ATOM	2603	CA	VAL	B	27	67.124	97.891	16.200	1.00	29.71	B
ATOM	2604	CB	VAL	B	27	68.507	97.703	16.858	1.00	36.67	B
ATOM	2605	CG1	VAL	B	27	68.477	96.507	17.808	1.00	31.87	B
ATOM	2606	CG2	VAL	B	27	69.564	97.478	15.793	1.00	32.00	B
ATOM	2607	C	VAL	B	27	66.054	97.946	17.292	1.00	26.09	B
ATOM	2608	O	VAL	B	27	65.961	98.921	18.029	1.00	28.74	B
ATOM	2609	N	ILE	B	28	65.230	96.913	17.349	1.00	28.74	B
ATOM	2610	CA	ILE	B	28	64.129	96.780	18.294	1.00	34.25	B
ATOM	2611	CB	ILE	B	28	62.802	96.400	17.552	1.00	38.10	B
ATOM	2612	CG2	ILE	B	28	61.751	95.929	18.516	1.00	49.78	B
ATOM	2613	CG1	ILE	B	28	62.260	97.598	16.808	1.00	46.71	B
ATOM	2614	CD1	ILE	B	28	62.253	98.826	17.612	1.00	40.93	B
ATOM	2615	C	ILE	B	28	64.491	95.619	19.223	1.00	38.36	B
ATOM	2616	O	ILE	B	28	65.063	94.626	18.769	1.00	29.90	B
ATOM	2617	N	ARG	B	29	64.134	95.724	20.503	1.00	30.42	B
ATOM	2618	CA	ARG	B	29	64.470	94.673	21.458	1.00	32.43	B
ATOM	2619	CB	ARG	B	29	65.468	95.242	22.461	1.00	38.54	B
ATOM	2620	CG	ARG	B	29	65.234	94.231	23.273	1.00	56.74	B
ATOM	2621	CD	ARG	B	29	67.479	94.939	23.821	1.00	68.43	B
ATOM	2622	NE	ARG	B	29	68.219	95.573	22.722	1.00	77.31	B
ATOM	2623	CZ	ARG	B	29	69.134	94.960	21.983	1.00	81.82	B
ATOM	2624	NH1	ARG	B	29	69.454	93.693	22.237	1.00	82.00	B
ATOM	2625	NH2	ARG	B	29	69.723	95.603	20.976	1.00	82.81	B
ATOM	2626	C	ARG	B	29	63.222	94.132	22.168	1.00	26.06	B
ATOM	2627	O	ARG	B	29	62.432	94.884	22.704	1.00	20.11	B
ATOM	2628	N	TYR	B	30	62.012	92.823	22.133	1.00	22.95	B
ATOM	2629	CA	TYR	B	30	61.886	92.206	22.787	1.00	31.30	B
ATOM	2630	CB	TYR	B	30	61.299	91.096	21.905	1.00	28.61	B
ATOM	2631	CG	TYR	B	30	60.647	91.547	20.605	1.00	29.37	B
ATOM	2632	CD1	TYR	B	30	61.339	92.135	19.579	1.00	24.77	B
ATOM	2633	CE1	TYR	B	30	60.781	92.553	18.387	1.00	19.11	B
ATOM	2634	CD2	TYR	B	30	59.282	91.378	20.403	1.00	29.03	B
ATOM	2635	CE2	TYR	B	30	58.674	91.785	19.215	1.00	26.35	B
ATOM	2636	CZ	TYR	B	30	59.429	92.379	18.216	1.00	23.41	B

ATOM	2637	OH	TYR	B	30	58.793	92.836	17.083	1.00	26.05	B
ATOM	2638	C	TYR	B	30	62.340	91.579	24.126	1.00	28.93	B
ATOM	2639	O	TYR	B	30	63.497	91.168	24.283	1.00	24.49	B
ATOM	2640	N	SER	B	31	61.418	91.488	25.067	1.00	26.50	B
ATOM	2641	CA	SER	B	31	61.697	90.903	26.369	1.00	24.95	B
ATOM	2642	CB	SER	B	31	62.304	91.946	27.308	1.00	21.32	B
ATOM	2643	OG	SER	B	31	61.426	93.028	27.483	1.00	26.55	B
ATOM	2644	C	SER	B	31	60.388	90.378	26.954	1.00	29.25	B
ATOM	2645	O	SER	B	31	59.287	90.780	26.529	1.00	22.45	B
ATOM	2646	N	CYS	B	32	60.515	89.484	27.930	1.00	27.99	B
ATOM	2647	CA	CYS	B	32	59.364	88.868	28.606	1.00	32.41	B
ATOM	2648	C	CYS	B	32	59.371	89.122	30.121	1.00	38.37	B
ATOM	2649	O	CYS	B	32	60.431	89.311	30.719	1.00	37.82	B
ATOM	2650	CB	CYS	B	32	59.371	87.347	28.400	1.00	30.70	B
ATOM	2651	SG	CYS	B	32	59.450	86.770	26.677	1.00	32.11	B
ATOM	2652	N	SER	B	33	58.178	89.101	30.717	1.00	51.37	B
ATOM	2653	CA	SER	B	33	57.995	89.265	32.163	1.00	56.15	B
ATOM	2654	CB	SER	B	33	56.544	89.013	32.552	1.00	60.18	B
ATOM	2655	OG	SER	B	33	55.675	89.714	31.672	1.00	66.23	B
ATOM	2656	C	SER	B	33	58.859	88.260	32.894	1.00	57.27	B
ATOM	2657	O	SER	B	33	59.535	87.427	32.274	1.00	60.30	B
ATOM	2658	N	GLY	B	34	58.805	88.290	34.219	1.00	53.29	B
ATOM	2659	CA	GLY	B	34	59.662	87.381	34.976	1.00	47.70	B
ATOM	2660	C	GLY	B	34	59.278	85.922	34.987	1.00	44.48	B
ATOM	2661	O	GLY	B	34	60.129	85.033	35.135	1.00	38.34	B
ATOM	2662	N	THR	B	35	57.993	85.660	34.818	1.00	40.51	B
ATOM	2663	CA	THR	B	35	57.524	84.290	34.860	1.00	40.76	B
ATOM	2664	CB	THR	B	35	56.225	84.279	35.644	1.00	41.73	B
ATOM	2665	OG1	THR	B	35	55.258	85.077	35.014	1.00	48.51	B
ATOM	2666	CG2	THR	B	35	56.468	84.761	37.057	1.00	44.89	B
ATOM	2667	C	THR	B	35	57.369	83.644	33.470	1.00	39.51	B
ATOM	2668	O	THR	B	35	56.786	82.613	33.086	1.00	31.97	B
ATOM	2669	N	PHE	B	36	57.924	84.349	32.491	1.00	35.56	B
ATOM	2670	CA	PHE	B	36	57.873	83.955	31.112	1.00	31.01	B
ATOM	2671	CB	PHE	B	36	57.116	84.967	30.250	1.00	33.05	B
ATOM	2672	CG	PHE	B	36	55.673	84.918	30.396	1.00	35.23	B
ATOM	2673	CD1	PHE	B	36	55.040	85.573	31.444	1.00	35.53	B
ATOM	2674	CD2	PHE	B	36	54.909	84.204	29.483	1.00	31.53	B
ATOM	2675	CE1	PHE	B	36	53.663	85.447	31.570	1.00	37.58	B
ATOM	2676	CE2	PHE	B	36	53.549	84.126	29.604	1.00	32.60	B
ATOM	2677	CZ	PHE	B	36	52.918	84.769	30.638	1.00	32.38	B
ATOM	2678	C	PHE	B	36	59.276	83.798	30.577	1.00	32.83	B
ATOM	2679	O	PHE	B	36	60.212	84.347	31.125	1.00	33.40	B
ATOM	2680	N	ARG	B	37	59.427	83.049	29.498	1.00	30.99	B
ATOM	2681	CA	ARG	B	37	60.741	82.849	28.916	1.00	29.69	B
ATOM	2682	CB	ARG	B	37	61.207	81.458	29.083	1.00	30.62	B
ATOM	2683	CG	ARG	B	37	61.442	81.072	30.541	1.00	35.61	B
ATOM	2684	CD	ARG	B	37	62.490	81.992	31.177	1.00	39.39	B
ATOM	2685	NE	ARG	B	37	62.303	82.044	32.629	1.00	49.28	B
ATOM	2686	CZ	ARG	B	37	62.847	81.168	33.451	1.00	47.41	B
ATOM	2687	NH1	ARG	B	37	63.614	80.210	32.947	1.00	53.00	B
ATOM	2688	NH2	ARG	B	37	62.602	81.223	34.751	1.00	44.10	B
ATOM	2689	C	ARG	B	37	60.713	83.280	27.439	1.00	32.05	B
ATOM	2690	O	ARG	B	37	59.809	82.874	26.700	1.00	25.63	B
ATOM	2691	N	LEU	B	38	61.706	84.050	27.011	1.00	23.96	B

ATOM	2692	CA	LEU	B	38	61.802	84.470	25.621	1.00	30.62	B
ATOM	2693	CB	LEU	B	38	62.655	85.738	25.508	1.00	23.25	B
ATOM	2694	CG	LEU	B	38	62.739	86.365	24.105	1.00	28.16	B
ATOM	2695	CD1	LEU	B	38	61.376	86.948	23.659	1.00	20.01	B
ATOM	2696	CD2	LEU	B	38	63.753	87.486	24.132	1.00	32.19	B
ATOM	2697	C	LEU	B	38	62.386	83.361	24.745	1.00	27.63	B
ATOM	2698	O	LEU	B	38	63.447	82.793	25.036	1.00	27.98	B
ATOM	2699	N	ILE	B	39	61.651	83.017	23.691	1.00	30.18	B
ATOM	2700	CA	ILE	B	39	62.073	81.983	22.743	1.00	27.37	B
ATOM	2701	CB	ILE	B	39	60.940	80.959	22.492	1.00	30.75	B
ATOM	2702	CG2	ILE	B	39	61.438	79.878	21.538	1.00	29.27	B
ATOM	2703	CG1	ILE	B	39	60.455	80.359	23.822	1.00	30.90	B
ATOM	2704	CD1	ILE	B	39	61.491	79.535	24.559	1.00	26.44	B
ATOM	2705	C	ILE	B	39	62.403	82.668	21.418	1.00	29.53	B
ATOM	2706	O	ILE	B	39	61.510	83.256	20.797	1.00	24.87	B
ATOM	2707	N	GLY	B	40	63.676	82.609	20.998	1.00	21.97	B
ATOM	2708	CA	GLY	B	40	64.084	83.239	19.751	1.00	23.62	B
ATOM	2709	C	GLY	B	40	64.957	84.450	19.975	1.00	22.85	B
ATOM	2710	O	GLY	B	40	65.065	84.921	21.104	1.00	21.42	B
ATOM	2711	N	GLU	B	41	65.592	84.958	18.925	1.00	27.33	B
ATOM	2712	CA	GLU	B	41	66.472	86.133	19.065	1.00	29.50	B
ATOM	2713	CB	GLU	B	41	67.138	86.471	17.730	1.00	33.78	B
ATOM	2714	CG	GLU	B	41	68.634	86.193	17.721	1.00	52.17	B
ATOM	2715	CD	GLU	B	41	69.411	87.123	18.648	1.00	57.74	B
ATOM	2716	OE1	GLU	B	41	70.414	86.641	19.231	1.00	66.30	B
ATOM	2717	OE2	GLU	B	41	69.034	88.326	18.791	1.00	53.76	B
ATOM	2718	C	GLU	B	41	65.667	87.333	19.541	1.00	30.40	B
ATOM	2719	O	GLU	B	41	64.601	87.619	18.995	1.00	27.22	B
ATOM	2720	N	LYS	B	42	66.197	88.049	20.528	1.00	27.86	B
ATOM	2721	CA	LYS	B	42	65.538	89.215	21.135	1.00	32.03	B
ATOM	2722	CB	LYS	B	42	66.171	89.495	22.504	1.00	37.19	B
ATOM	2723	CG	LYS	B	42	67.610	89.990	22.379	1.00	43.78	B
ATOM	2724	CD	LYS	B	42	68.196	90.536	23.674	1.00	54.68	B
ATOM	2725	CE	LYS	B	42	68.055	89.538	24.812	1.00	62.51	B
ATOM	2726	NZ	LYS	B	42	68.438	88.139	24.443	1.00	69.20	B
ATOM	2727	C	LYS	B	42	65.586	90.530	20.331	1.00	32.32	B
ATOM	2728	O	LYS	B	42	64.771	91.432	20.535	1.00	27.61	B
ATOM	2729	N	SER	B	43	66.547	90.680	19.423	1.00	28.99	B
ATOM	2730	CA	SER	B	43	66.611	91.946	18.672	1.00	33.61	B
ATOM	2731	CB	SER	B	43	68.012	92.565	18.722	1.00	29.97	B
ATOM	2732	OG	SER	B	43	68.478	92.606	20.047	1.00	47.21	B
ATOM	2733	C	SER	B	43	66.273	91.770	17.224	1.00	28.57	B
ATOM	2734	O	SER	B	43	66.765	90.841	16.588	1.00	32.11	B
ATOM	2735	N	LEU	B	44	65.443	92.661	16.697	1.00	26.09	B
ATOM	2736	CA	LEU	B	44	65.127	92.607	15.280	1.00	25.34	B
ATOM	2737	CB	LEU	B	44	63.620	92.609	14.987	1.00	21.75	B
ATOM	2738	CG	LEU	B	44	62.608	91.642	15.595	1.00	33.26	B
ATOM	2739	CD1	LEU	B	44	61.455	91.187	14.626	1.00	24.66	B
ATOM	2740	CD2	LEU	B	44	63.227	90.293	15.976	1.00	19.72	B
ATOM	2741	C	LEU	B	44	65.738	93.863	14.694	1.00	27.39	B
ATOM	2742	O	LEU	B	44	65.759	94.919	15.334	1.00	29.07	B
ATOM	2743	N	LEU	B	45	66.201	93.740	13.456	1.00	26.79	B
ATOM	2744	CA	LEU	B	45	66.854	94.812	12.727	1.00	26.17	B
ATOM	2745	CB	LEU	B	45	68.202	94.303	12.213	1.00	25.36	B
ATOM	2746	CG	LEU	B	45	69.343	95.281	11.950	1.00	35.90	B

ATOM	2747	CD1	LEU	B	45	70.263	94.668	10.905	1.00	31.78	B
ATOM	2748	CD2	LEU	B	45	68.853	96.627	11.519	1.00	33.62	B
ATOM	2749	C	LEU	B	45	66.016	95.198	11.516	1.00	25.11	B
ATOM	2750	O	LEU	B	45	65.568	94.320	10.761	1.00	20.94	B
ATOM	2751	N	CYS	B	46	65.803	96.487	11.298	1.00	24.35	B
ATOM	2752	CA	CYS	B	46	65.057	96.887	10.097	1.00	22.87	B
ATOM	2753	C	CYS	B	46	66.106	96.897	8.976	1.00	29.24	B
ATOM	2754	O	CYS	B	46	67.099	97.601	9.051	1.00	28.56	B
ATOM	2755	CB	CYS	B	46	64.446	98.284	10.251	1.00	26.50	B
ATOM	2756	SG	CYS	B	46	63.677	98.900	8.705	1.00	27.31	B
ATOM	2757	N	ILE	B	47	65.877	96.106	7.943	1.00	24.65	B
ATOM	2758	CA	ILE	B	47	66.817	95.991	6.842	1.00	28.64	B
ATOM	2759	CB	ILE	B	47	67.412	94.572	6.871	1.00	30.17	B
ATOM	2760	CG2	ILE	B	47	68.114	94.258	5.601	1.00	42.28	B
ATOM	2761	CG1	ILE	B	47	68.341	94.458	8.070	1.00	40.16	B
ATOM	2762	CD1	ILE	B	47	69.121	93.190	8.107	1.00	53.27	B
ATOM	2763	C	ILE	B	47	66.098	96.188	5.504	1.00	28.32	B
ATOM	2764	O	ILE	B	47	64.874	96.332	5.466	1.00	24.70	B
ATOM	2765	N	THR	B	48	66.853	96.238	4.413	1.00	24.30	B
ATOM	2766	CA	THR	B	48	66.236	96.267	3.091	1.00	27.24	B
ATOM	2767	CB	THR	B	48	66.215	97.672	2.405	1.00	31.04	B
ATOM	2768	OG1	THR	B	48	65.632	97.534	1.090	1.00	26.58	B
ATOM	2769	CG2	THR	B	48	67.627	98.250	2.271	1.00	25.54	B
ATOM	2770	C	THR	B	48	67.048	95.280	2.254	1.00	26.55	B
ATOM	2771	O	THR	B	48	68.276	95.371	2.173	1.00	27.30	B
ATOM	2772	N	LYS	B	49	66.370	94.295	1.688	1.00	24.39	B
ATOM	2773	CA	LYS	B	49	67.031	93.309	0.837	1.00	25.65	B
ATOM	2774	CB	LYS	B	49	66.323	91.943	0.940	1.00	27.44	B
ATOM	2775	CG	LYS	B	49	66.358	91.351	2.368	1.00	36.21	B
ATOM	2776	CD	LYS	B	49	67.171	90.103	2.479	1.00	43.52	B
ATOM	2777	CE	LYS	B	49	68.570	90.294	2.025	1.00	41.66	B
ATOM	2778	NZ	LYS	B	49	69.314	89.069	2.403	1.00	46.47	B
ATOM	2779	C	LYS	B	49	67.041	93.752	-0.632	1.00	33.01	B
ATOM	2780	O	LYS	B	49	67.987	93.450	-1.353	1.00	26.70	B
ATOM	2781	N	ASP	B	50	65.994	94.451	-1.083	1.00	26.02	B
ATOM	2782	CA	ASP	B	50	65.933	94.859	-2.495	1.00	29.77	B
ATOM	2783	CB	ASP	B	50	64.575	94.503	-3.108	1.00	28.00	B
ATOM	2784	CG	ASP	B	50	63.439	95.221	-2.440	1.00	26.54	B
ATOM	2785	OD1	ASP	B	50	63.720	96.043	-1.562	1.00	25.74	B
ATOM	2786	OD2	ASP	B	50	62.262	94.969	-2.779	1.00	32.42	B
ATOM	2787	C	ASP	B	50	66.200	96.327	-2.744	1.00	30.62	B
ATOM	2788	O	ASP	B	50	66.037	96.794	-3.858	1.00	24.13	B
ATOM	2789	N	LYS	B	51	66.610	97.050	-1.709	1.00	27.94	B
ATOM	2790	CA	LYS	B	51	66.889	98.473	-1.824	1.00	31.18	B
ATOM	2791	CB	LYS	B	51	68.014	98.742	-2.819	1.00	34.46	B
ATOM	2792	CG	LYS	B	51	69.381	98.355	-2.297	1.00	41.85	B
ATOM	2793	CD	LYS	B	51	70.447	98.960	-3.175	1.00	48.97	B
ATOM	2794	CE	LYS	B	51	71.826	98.869	-2.564	1.00	54.90	B
ATOM	2795	NZ	LYS	B	51	72.751	99.713	-3.366	1.00	67.70	B
ATOM	2796	C	LYS	B	51	65.666	99.305	-2.186	1.00	30.97	B
ATOM	2797	O	LYS	B	51	65.786	100.430	-2.634	1.00	28.68	B
ATOM	2798	N	VAL	B	52	64.483	98.748	-1.992	1.00	26.95	B
ATOM	2799	CA	VAL	B	52	63.263	99.501	-2.231	1.00	26.37	B
ATOM	2800	CB	VAL	B	52	62.456	98.945	-3.402	1.00	27.69	B
ATOM	2801	CG1	VAL	B	52	61.123	99.695	-3.511	1.00	32.70	B

ATOM	2802	CG2	VAL	B	52	63.236	99.113	-4.679	1.00	32.13	B
ATOM	2803	C	VAL	B	52	62.375	99.437	-1.000	1.00	30.79	B
ATOM	2804	O	VAL	B	52	61.949	100.461	-0.491	1.00	26.76	B
ATOM	2805	N	ASP	B	53	62.102	98.232	-0.512	1.00	26.86	B
ATOM	2806	CA	ASP	B	53	61.210	98.074	0.642	1.00	26.94	B
ATOM	2807	CB	ASP	B	53	60.156	96.999	0.318	1.00	42.02	B
ATOM	2808	CG	ASP	B	53	59.285	97.356	-0.871	1.00	53.53	B
ATOM	2809	OD1	ASP	B	53	58.878	98.540	-0.943	1.00	63.13	B
ATOM	2810	OD2	ASP	B	53	58.964	96.476	-1.727	1.00	64.13	B
ATOM	2811	C	ASP	B	53	62.006	97.651	1.888	1.00	25.00	B
ATOM	2812	O	ASP	B	53	63.063	97.038	1.773	1.00	22.23	B
ATOM	2813	N	GLY	B	54	61.490	97.959	3.072	1.00	20.64	B
ATOM	2814	CA	GLY	B	54	62.170	97.578	4.293	1.00	24.10	B
ATOM	2815	C	GLY	B	54	61.441	96.397	4.919	1.00	25.17	B
ATOM	2816	O	GLY	B	54	60.237	96.266	4.728	1.00	25.23	B
ATOM	2817	N	THR	B	55	62.169	95.517	5.605	1.00	23.87	B
ATOM	2818	CA	THR	B	55	61.589	94.373	6.318	1.00	20.36	B
ATOM	2819	CB	THR	B	55	61.679	93.051	5.518	1.00	27.74	B
ATOM	2820	OG1	THR	B	55	61.052	92.004	6.267	1.00	24.11	B
ATOM	2821	CG2	THR	B	55	63.151	92.669	5.212	1.00	21.92	B
ATOM	2822	C	THR	B	55	62.371	94.156	7.600	1.00	22.54	B
ATOM	2823	O	THR	B	55	63.535	94.526	7.675	1.00	24.57	B
ATOM	2824	N	TRP	B	56	61.743	93.589	8.624	1.00	23.11	B
ATOM	2825	CA	TRP	B	56	62.513	93.285	9.827	1.00	25.54	B
ATOM	2826	CB	TRP	B	56	61.580	92.954	10.988	1.00	23.18	B
ATOM	2827	CG	TRP	B	56	60.874	94.202	11.420	1.00	19.51	B
ATOM	2828	CD2	TRP	B	56	61.456	95.282	12.147	1.00	21.91	B
ATOM	2829	CE2	TRP	B	56	60.473	96.302	12.247	1.00	26.89	B
ATOM	2830	CE3	TRP	B	56	62.722	95.491	12.729	1.00	25.30	B
ATOM	2831	CD1	TRP	B	56	59.595	94.578	11.119	1.00	21.93	B
ATOM	2832	NE1	TRP	B	56	59.343	95.849	11.617	1.00	21.49	B
ATOM	2833	CZ2	TRP	B	56	60.713	97.521	12.895	1.00	26.71	B
ATOM	2834	CZ3	TRP	B	56	62.963	96.706	13.380	1.00	29.35	B
ATOM	2835	CH2	TRP	B	56	61.957	97.706	13.451	1.00	28.96	B
ATOM	2836	C	TRP	B	56	63.335	92.075	9.384	1.00	28.11	B
ATOM	2837	O	TRP	B	56	62.882	91.296	8.535	1.00	23.54	B
ATOM	2838	N	ASP	B	57	64.535	91.909	9.926	1.00	20.44	B
ATOM	2839	CA	ASP	B	57	65.401	90.812	9.470	1.00	25.81	B
ATOM	2840	CB	ASP	B	57	66.885	91.113	9.761	1.00	30.15	B
ATOM	2841	CG	ASP	B	57	67.234	91.045	11.255	1.00	35.84	B
ATOM	2842	OD1	ASP	B	57	66.319	91.161	12.102	1.00	23.31	B
ATOM	2843	OD2	ASP	B	57	68.443	90.889	11.581	1.00	41.06	B
ATOM	2844	C	ASP	B	57	65.058	89.433	9.963	1.00	26.11	B
ATOM	2845	O	ASP	B	57	65.634	88.455	9.486	1.00	28.90	B
ATOM	2846	N	LYS	B	58	64.114	89.336	10.896	1.00	29.91	B
ATOM	2847	CA	LYS	B	58	63.687	88.032	11.411	1.00	27.97	B
ATOM	2848	CB	LYS	B	58	64.697	87.491	12.443	1.00	30.61	B
ATOM	2849	CG	LYS	B	58	64.884	88.378	13.650	1.00	38.24	B
ATOM	2850	CD	LYS	B	58	65.966	87.831	14.618	1.00	41.02	B
ATOM	2851	CE	LYS	B	58	67.406	88.063	14.115	1.00	37.73	B
ATOM	2852	NZ	LYS	B	58	67.830	89.511	14.119	1.00	29.19	B
ATOM	2853	C	LYS	B	58	62.319	88.105	12.045	1.00	22.71	B
ATOM	2854	O	LYS	B	58	61.795	89.188	12.311	1.00	26.33	B
ATOM	2855	N	PRO	B	59	61.700	86.947	12.292	1.00	25.99	B
ATOM	2856	CD	PRO	B	59	62.084	85.584	11.885	1.00	24.09	B

ATOM	2857	CA	PRO	B	59	60.367	86.972	12.919	1.00	22.11	B
ATOM	2858	CB	PRO	B	59	59.902	85.515	12.845	1.00	26.86	B
ATOM	2859	CG	PRO	B	59	60.730	84.913	11.746	1.00	29.91	B
ATOM	2860	C	PRO	B	59	62.304	87.419	14.369	1.00	30.21	B
ATOM	2861	O	PRO	B	59	61.394	87.307	14.968	1.00	28.15	B
ATOM	2862	N	ALA	B	60	59.433	87.924	14.951	1.00	25.43	B
ATOM	2863	CA	ALA	B	60	59.516	88.330	16.339	1.00	26.37	B
ATOM	2864	CB	ALA	B	60	58.260	89.089	16.742	1.00	26.63	B
ATOM	2865	C	ALA	B	60	59.644	87.085	17.223	1.00	21.91	B
ATOM	2866	O	ALA	B	60	59.104	86.068	16.914	1.00	22.47	B
ATOM	2867	N	PRO	B	61	60.353	87.173	18.350	1.00	23.37	B
ATOM	2868	CD	PRO	B	61	61.134	88.320	18.870	1.00	22.24	B
ATOM	2869	CA	PRO	B	61	60.476	86.007	19.227	1.00	19.99	B
ATOM	2870	CB	PRO	B	61	61.650	86.386	20.130	1.00	21.18	B
ATOM	2871	CG	PRO	B	61	61.458	87.876	20.314	1.00	22.73	B
ATOM	2872	C	PRO	B	61	59.151	85.933	20.024	1.00	27.42	B
ATOM	2873	O	PRO	B	61	58.314	86.831	19.903	1.00	27.48	B
ATOM	2874	N	LYS	B	62	58.960	84.893	20.834	1.00	21.73	B
ATOM	2875	CA	LYS	B	62	57.737	84.770	21.648	1.00	26.90	B
ATOM	2876	CB	LYS	B	62	56.980	83.576	21.187	1.00	32.90	B
ATOM	2877	CG	LYS	B	62	56.316	83.743	19.779	1.00	39.12	B
ATOM	2878	CD	LYS	B	62	55.638	82.502	19.258	1.00	48.29	B
ATOM	2879	CE	LYS	B	62	55.142	82.741	17.828	1.00	54.55	B
ATOM	2880	NZ	LYS	B	62	54.620	81.478	17.213	1.00	59.87	B
ATOM	2881	C	LYS	B	62	58.050	84.601	23.133	1.00	30.68	B
ATOM	2882	O	LYS	B	62	59.190	84.287	23.528	1.00	24.62	B
ATOM	2883	N	CYS	B	63	57.039	84.843	23.958	1.00	25.15	B
ATOM	2884	CA	CYS	B	63	57.171	84.675	25.405	1.00	27.27	B
ATOM	2885	C	CYS	B	63	55.814	83.481	25.792	1.00	30.43	B
ATOM	2886	O	CYS	B	63	55.111	83.454	25.515	1.00	30.82	B
ATOM	2887	CB	CYS	B	63	56.646	85.903	26.149	1.00	25.60	B
ATOM	2888	SG	CYS	B	63	57.685	87.384	25.922	1.00	31.81	B
ATOM	2889	N	GLU	B	64	56.734	82.486	26.414	1.00	29.14	B
ATOM	2890	CA	GLU	B	64	56.220	81.297	26.871	1.00	27.87	B
ATOM	2891	CB	GLU	B	64	56.938	80.043	26.393	1.00	22.54	B
ATOM	2892	CG	GLU	B	64	56.939	79.836	24.884	1.00	30.23	B
ATOM	2893	CD	GLU	B	64	57.354	78.472	24.471	1.00	25.42	B
ATOM	2894	OE1	GLU	B	64	56.146	77.879	25.221	1.00	28.63	B
ATOM	2895	OE2	GLU	B	64	56.993	77.994	23.396	1.00	24.45	B
ATOM	2896	C	GLU	B	64	54.172	81.301	28.394	1.00	27.43	B
ATOM	2897	O	GLU	B	64	53.184	81.564	29.036	1.00	28.45	B
ATOM	2898	N	TYR	B	65	54.006	81.039	28.981	1.00	30.82	B
ATOM	2899	CA	TYR	B	65	52.998	81.016	30.449	1.00	26.71	B
ATOM	2900	CB	TYR	B	65	53.474	80.638	30.881	1.00	24.97	B
ATOM	2901	CG	TYR	B	65	53.224	81.754	32.382	1.00	30.61	B
ATOM	2902	CD1	TYR	B	65	53.958	81.915	33.078	1.00	37.93	B
ATOM	2903	CE1	TYR	B	65	53.764	82.913	34.464	1.00	37.10	B
ATOM	2904	CD2	TYR	B	65	52.681	79.689	33.102	1.00	29.91	B
ATOM	2905	CE2	TYR	B	65	52.481	79.765	34.477	1.00	32.04	B
ATOM	2906	CZ	TYR	B	65	52.829	80.927	35.149	1.00	38.91	B
ATOM	2907	OH	TYR	B	65	52.653	81.014	36.510	1.00	40.82	B
ATOM	2908	C	TYR	B	65	55.931	79.069	30.908	1.00	26.37	B
ATOM	2909	O	TYR	B	65	56.022	78.891	30.339	1.00	27.39	B
ATOM	2910	N	PHE	B	66	56.722	80.290	31.924	1.00	30.93	B
ATOM	2911	CA	PHE	B	66	57.770	79.381	32.362	1.00	29.14	B

ATOM	2912	CB	PHE	B	66	58.611	80.060	33.455	1.00	27.56	B
ATOM	2913	CG	PHE	B	66	59.743	79.210	33.998	1.00	28.67	B
ATOM	2914	CD1	PHE	B	66	60.632	78.559	33.139	1.00	33.68	B
ATOM	2915	CD2	PHE	B	66	59.907	79.055	35.371	1.00	30.48	B
ATOM	2916	CE1	PHE	B	66	61.669	77.763	33.648	1.00	35.23	B
ATOM	2917	CE2	PHE	B	66	60.931	78.267	35.895	1.00	26.93	B
ATOM	2918	CZ	PHE	B	66	61.816	77.618	35.041	1.00	31.25	B
ATOM	2919	C	PHE	B	66	57.283	78.013	32.844	1.00	32.09	B
ATOM	2920	O	PHE	B	66	56.382	77.924	33.671	1.00	31.84	B
ATOM	2921	N	ASN	B	67	57.882	76.956	32.312	1.00	28.91	B
ATOM	2922	CA	ASN	B	67	57.553	75.591	32.727	1.00	31.14	B
ATOM	2923	CB	ASN	B	67	57.124	74.763	31.524	1.00	32.40	B
ATOM	2924	CG	ASN	B	67	56.635	73.363	31.903	1.00	37.56	B
ATOM	2925	OD1	ASN	B	67	57.193	72.701	32.784	1.00	33.77	B
ATOM	2926	ND2	ASN	B	67	55.589	72.914	31.218	1.00	40.31	B
ATOM	2927	C	ASN	B	67	58.844	75.009	33.318	1.00	30.31	B
ATOM	2928	O	ASN	B	67	59.719	74.551	32.577	1.00	26.39	B
ATOM	2929	N	LYS	B	68	58.960	75.038	34.644	1.00	28.27	B
ATOM	2930	CA	LYS	B	68	60.148	74.535	35.329	1.00	29.00	B
ATOM	2931	CB	LYS	B	68	60.041	74.792	36.843	1.00	35.08	B
ATOM	2932	CG	LYS	B	68	58.984	73.906	37.518	1.00	41.56	B
ATOM	2933	CD	LYS	B	68	59.179	73.778	39.031	1.00	52.33	B
ATOM	2934	CE	LYS	B	68	58.907	75.077	39.764	1.00	54.82	B
ATOM	2935	NZ	LYS	B	68	58.896	74.891	41.250	1.00	58.88	B
ATOM	2936	C	LYS	B	68	60.398	73.039	35.087	1.00	32.74	B
ATOM	2937	O	LYS	B	68	61.507	72.556	35.318	1.00	32.92	B
ATOM	2938	N	TYR	B	69	59.389	72.305	34.611	1.00	33.19	B
ATOM	2939	CA	TYR	B	69	59.569	70.867	34.354	1.00	25.62	B
ATOM	2940	CB	TYR	B	69	58.259	70.096	34.687	1.00	30.97	B
ATOM	2941	CG	TYR	B	69	57.301	70.349	36.107	1.00	30.82	B
ATOM	2942	CD1	TYR	B	69	56.774	71.264	36.378	1.00	28.48	B
ATOM	2943	CE1	TYR	B	69	56.444	71.623	37.697	1.00	31.73	B
ATOM	2944	CD2	TYR	B	69	58.486	69.776	37.192	1.00	31.64	B
ATOM	2945	CE2	TYR	B	69	58.174	70.118	38.507	1.00	38.99	B
ATOM	2946	CZ	TYR	B	69	57.153	71.053	38.756	1.00	39.94	B
ATOM	2947	OH	TYR	B	69	56.901	71.467	40.043	1.00	41.68	B
ATOM	2948	C	TYR	B	69	60.023	70.516	32.955	1.00	31.61	B
ATOM	2949	O	TYR	B	69	60.549	69.414	32.722	1.00	31.53	B
ATOM	2950	N	SER	B	70	59.389	71.447	32.017	1.00	29.13	B
ATOM	2951	CA	SER	B	70	60.328	71.162	30.649	1.00	31.79	B
ATOM	2952	CB	SER	B	70	59.926	72.310	29.708	1.00	27.84	B
ATOM	2953	OG	SER	B	70	58.524	72.534	29.725	1.00	38.42	B
ATOM	2954	C	SER	B	70	61.849	70.949	30.544	1.00	34.24	B
ATOM	2955	O	SER	B	70	62.624	71.534	31.296	1.00	31.38	B
ATOM	2956	N	SER	B	71	62.261	70.097	29.613	1.00	33.64	B
ATOM	2957	CA	SER	B	71	63.679	69.832	29.351	1.00	36.09	B
ATOM	2958	CB	SER	B	71	64.265	68.809	30.324	1.00	39.34	B
ATOM	2959	OG	SER	B	71	63.823	67.519	30.007	1.00	41.01	B
ATOM	2960	C	SER	B	71	63.736	69.308	27.907	1.00	41.17	B
ATOM	2961	O	SER	B	71	62.959	68.520	27.432	1.00	41.30	B
ATOM	2962	N	CYS	B	72	64.805	69.766	27.195	1.00	32.35	B
ATOM	2963	CA	CYS	B	72	64.970	69.351	25.816	1.00	36.35	B
ATOM	2964	C	CYS	B	72	66.139	68.393	25.722	1.00	36.24	B
ATOM	2965	O	CYS	B	72	67.039	68.472	26.503	1.00	34.41	B
ATOM	2966	CB	CYS	B	72	65.205	70.586	24.920	1.00	26.09	B

ATOM	2967	SG	CYS	B	72	63.836	71.795	24.962	1.00	32.64	B
ATOM	2968	N	PRO	B	73	66.069	67.453	24.779	1.00	35.65	B
ATOM	2969	CD	PRO	B	73	64.958	67.148	23.867	1.00	38.10	B
ATOM	2970	CA	PRO	B	73	67.157	66.494	24.617	1.00	35.61	B
ATOM	2971	CB	PRO	B	73	66.567	65.461	23.661	1.00	35.75	B
ATOM	2972	CG	PRO	B	73	65.662	66.314	22.806	1.00	40.23	B
ATOM	2973	C	PRO	B	73	68.355	67.203	24.011	1.00	37.18	B
ATOM	2974	O	PRO	B	73	68.225	68.277	23.427	1.00	31.86	B
ATOM	2975	N	GLU	B	74	69.521	66.595	24.151	1.00	30.08	B
ATOM	2976	CA	GLU	B	74	70.726	67.168	23.594	1.00	36.66	B
ATOM	2977	CB	GLU	B	74	71.904	66.221	23.830	1.00	40.69	B
ATOM	2978	CG	GLU	B	74	73.123	66.500	22.972	1.00	55.61	B
ATOM	2979	CD	GLU	B	74	74.357	66.847	23.791	1.00	65.33	B
ATOM	2980	OE1	GLU	B	74	75.476	66.535	23.311	1.00	68.86	B
ATOM	2981	OE2	GLU	B	74	74.214	67.432	24.899	1.00	67.56	B
ATOM	2982	C	GLU	B	74	70.526	67.411	22.099	1.00	31.83	B
ATOM	2983	O	GLU	B	74	70.179	66.517	21.347	1.00	34.92	B
ATOM	2984	N	PRO	B	75	70.743	68.639	21.648	1.00	29.85	B
ATOM	2985	CD	PRO	B	75	71.019	69.851	22.431	1.00	29.21	B
ATOM	2986	CA	PRO	B	75	70.573	68.944	20.227	1.00	31.16	B
ATOM	2987	CB	PRO	B	75	70.349	70.441	20.235	1.00	30.77	B
ATOM	2988	CG	PRO	B	75	71.310	70.872	21.362	1.00	28.27	B
ATOM	2989	C	PRO	B	75	71.855	68.552	19.507	1.00	37.41	B
ATOM	2990	O	PRO	B	75	72.949	68.998	19.877	1.00	35.98	B
ATOM	2991	N	ILE	B	76	71.728	67.726	18.474	1.00	37.41	B
ATOM	2992	CA	ILE	B	76	72.904	67.277	17.757	1.00	41.40	B
ATOM	2993	CB	ILE	B	76	73.069	65.755	17.912	1.00	47.80	B
ATOM	2994	CG2	ILE	B	76	74.385	65.302	17.272	1.00	48.99	B
ATOM	2995	CG1	ILE	B	76	73.078	65.396	19.404	1.00	48.44	B
ATOM	2996	CD1	ILE	B	76	72.926	63.913	19.671	1.00	55.08	B
ATOM	2997	C	ILE	B	76	72.874	67.654	16.294	1.00	38.62	B
ATOM	2998	O	ILE	B	76	71.874	67.480	15.625	1.00	39.69	B
ATOM	2999	N	VAL	B	77	73.984	68.195	15.913	1.00	36.89	B
ATOM	3000	CA	VAL	B	77	74.107	68.610	14.433	1.00	38.30	B
ATOM	3001	CB	VAL	B	77	74.290	70.119	14.331	1.00	39.19	B
ATOM	3002	CG1	VAL	B	77	74.483	70.519	12.871	1.00	39.16	B
ATOM	3003	CG2	VAL	B	77	73.081	70.826	14.946	1.00	40.99	B
ATOM	3004	C	VAL	B	77	75.307	67.939	13.761	1.00	40.36	B
ATOM	3005	O	VAL	B	77	76.457	68.351	13.948	1.00	41.17	B
ATOM	3006	N	PRO	B	78	75.057	66.893	12.966	1.00	40.75	B
ATOM	3007	CD	PRO	B	78	73.785	66.267	12.590	1.00	37.39	B
ATOM	3008	CA	PRO	B	78	76.183	66.228	12.303	1.00	40.96	B
ATOM	3009	CB	PRO	B	78	75.506	65.195	11.412	1.00	41.91	B
ATOM	3010	CG	PRO	B	78	74.119	65.745	11.229	1.00	45.49	B
ATOM	3011	C	PRO	B	78	76.997	67.232	11.525	1.00	37.80	B
ATOM	3012	O	PRO	B	78	76.447	68.140	10.913	1.00	37.38	B
ATOM	3013	N	GLY	B	79	78.312	67.083	11.590	1.00	32.94	B
ATOM	3014	CA	GLY	B	79	79.186	68.002	10.900	1.00	36.40	B
ATOM	3015	C	GLY	B	79	79.427	69.261	11.712	1.00	34.31	B
ATOM	3016	O	GLY	B	79	80.209	70.109	12.134	1.00	42.13	B
ATOM	3017	N	GLY	B	80	78.760	69.404	12.855	1.00	36.96	B
ATOM	3018	CA	GLY	B	80	78.960	70.608	13.664	1.00	39.25	B
ATOM	3019	C	GLY	B	80	79.072	70.348	15.164	1.00	35.08	B
ATOM	3020	O	GLY	B	80	78.994	69.202	15.609	1.00	40.28	B
ATOM	3021	N	TYR	B	81	79.225	71.410	15.953	1.00	37.65	B

ATOM	3022	CA	TYR	B	81	79.345	71.271	17.408	1.00	33.04	B
ATOM	3023	CB	TYR	B	81	80.800	71.019	17.799	1.00	29.39	B
ATOM	3024	CG	TYR	B	81	81.745	72.112	17.331	1.00	31.26	B
ATOM	3025	CD1	TYR	B	81	82.169	73.116	18.199	1.00	28.35	B
ATOM	3026	CE1	TYR	B	81	82.992	74.143	17.766	1.00	28.17	B
ATOM	3027	CD2	TYR	B	81	82.181	72.163	16.004	1.00	28.62	B
ATOM	3028	CE2	TYR	B	81	83.006	73.188	15.559	1.00	31.47	B
ATOM	3029	CZ	TYR	B	81	83.401	74.174	16.449	1.00	30.40	B
ATOM	3030	OH	TYR	B	81	84.172	75.207	16.012	1.00	32.87	B
ATOM	3031	C	TYR	B	81	78.847	72.536	18.095	1.00	33.96	B
ATOM	3032	O	TYR	B	81	78.696	73.581	17.454	1.00	30.79	B
ATOM	3033	N	LYS	B	82	78.600	72.431	19.398	1.00	23.56	B
ATOM	3034	CA	LYS	B	82	78.114	73.557	20.195	1.00	29.94	B
ATOM	3035	CB	LYS	B	82	77.348	73.034	21.428	1.00	25.29	B
ATOM	3036	CG	LYS	B	82	76.140	72.144	21.057	1.00	27.67	B
ATOM	3037	CD	LYS	B	82	75.335	71.652	22.266	1.00	33.47	B
ATOM	3038	CE	LYS	B	82	76.215	71.041	23.365	1.00	44.83	B
ATOM	3039	NZ	LYS	B	82	77.091	69.944	22.837	1.00	45.24	B
ATOM	3040	C	LYS	B	82	79.205	74.526	20.629	1.00	29.85	B
ATOM	3041	O	LYS	B	82	80.270	74.110	21.099	1.00	31.44	B
ATOM	3042	N	ILE	B	83	78.980	75.822	20.428	1.00	25.93	B
ATOM	3043	CA	ILE	B	83	79.959	76.795	20.887	1.00	21.30	B
ATOM	3044	CB	ILE	B	83	80.449	77.771	19.800	1.00	29.03	B
ATOM	3045	CG2	ILE	B	83	81.296	77.004	18.799	1.00	23.68	B
ATOM	3046	CG1	ILE	B	83	79.278	78.514	19.155	1.00	24.89	B
ATOM	3047	CD1	ILE	B	83	79.722	79.571	18.148	1.00	27.44	B
ATOM	3048	C	ILE	B	83	79.362	77.581	22.027	1.00	26.62	B
ATOM	3049	O	ILE	B	83	80.038	78.408	22.636	1.00	32.15	B
ATOM	3050	N	ARG	B	84	78.092	77.330	22.324	1.00	24.60	B
ATOM	3051	CA	ARG	B	84	77.471	77.981	23.469	1.00	25.74	B
ATOM	3052	CB	ARG	B	84	77.047	79.396	23.131	1.00	34.80	B
ATOM	3053	CG	ARG	B	84	76.583	80.160	24.348	1.00	45.89	B
ATOM	3054	CD	ARG	B	84	76.518	81.629	24.027	1.00	56.25	B
ATOM	3055	NE	ARG	B	84	77.801	82.302	24.217	1.00	60.31	B
ATOM	3056	CZ	ARG	B	84	78.276	82.707	25.397	1.00	64.61	B
ATOM	3057	NH1	ARG	B	84	77.581	82.496	26.512	1.00	66.21	B
ATOM	3058	NH2	ARG	B	84	79.421	83.386	25.454	1.00	61.85	B
ATOM	3059	C	ARG	B	84	76.278	77.199	23.384	1.00	27.61	B
ATOM	3060	O	ARG	B	84	75.487	76.687	23.189	1.00	24.27	B
ATOM	3061	N	GLY	B	85	76.166	77.105	25.314	1.00	25.11	B
ATOM	3062	CA	GLY	B	85	75.074	76.374	25.959	1.00	23.64	B
ATOM	3063	C	GLY	B	85	75.394	74.877	26.115	1.00	32.13	B
ATOM	3064	O	GLY	B	85	75.961	74.257	25.200	1.00	25.66	B
ATOM	3065	N	SER	B	86	75.094	74.293	27.281	1.00	24.97	B
ATOM	3066	CA	SER	B	86	75.347	72.859	27.473	1.00	34.32	B
ATOM	3067	CB	SER	B	86	76.755	72.588	28.034	1.00	31.54	B
ATOM	3068	OG	SER	B	86	76.964	73.322	29.223	1.00	47.05	B
ATOM	3069	C	SER	B	86	74.315	72.304	28.415	1.00	27.69	B
ATOM	3070	O	SER	B	86	73.536	73.064	28.979	1.00	24.75	B
ATOM	3071	N	THR	B	87	74.294	70.982	28.573	1.00	27.03	B
ATOM	3072	CA	THR	B	87	73.325	70.314	29.454	1.00	29.87	B
ATOM	3073	CB	THR	B	87	73.532	68.806	29.450	1.00	34.20	B
ATOM	3074	OG1	THR	B	87	73.876	68.395	28.125	1.00	54.47	B
ATOM	3075	CG2	THR	B	87	72.263	68.107	29.856	1.00	36.26	B
ATOM	3076	C	THR	B	87	73.420	70.767	30.903	1.00	30.09	B

ATOM	3077	O	THR	B	87	74.501	71.113	31.381	1.00	30.94	B
ATOM	3078	N	PRO	B	88	72.293	70.771	31.626	1.00	26.03	B
ATOM	3079	CD	PRO	B	88	72.370	71.088	33.060	1.00	30.64	B
ATOM	3080	CA	PRO	B	88	70.921	70.406	31.240	1.00	33.13	B
ATOM	3081	CB	PRO	B	88	70.225	70.211	32.585	1.00	28.86	B
ATOM	3082	CG	PRO	B	88	70.903	71.248	33.440	1.00	31.91	B
ATOM	3083	C	PRO	B	88	70.228	71.482	30.388	1.00	31.83	B
ATOM	3084	O	PRO	B	88	70.495	72.668	30.535	1.00	29.33	B
ATOM	3085	N	TYR	B	89	69.340	71.059	29.503	1.00	27.84	B
ATOM	3086	CA	TYR	B	89	68.613	71.990	28.641	1.00	29.55	B
ATOM	3087	CB	TYR	B	89	68.553	71.414	27.239	1.00	27.73	B
ATOM	3088	CG	TYR	B	89	69.938	71.078	26.722	1.00	29.87	B
ATOM	3089	CD1	TYR	B	89	70.326	69.759	26.501	1.00	33.12	B
ATOM	3090	CE1	TYR	B	89	71.605	69.456	26.036	1.00	26.70	B
ATOM	3091	CD2	TYR	B	89	70.865	72.086	26.467	1.00	32.19	B
ATOM	3092	CE2	TYR	B	89	72.134	71.795	26.007	1.00	28.60	B
ATOM	3093	CZ	TYR	B	89	72.492	70.482	25.802	1.00	27.81	B
ATOM	3094	OH	TYR	B	89	73.770	70.211	25.415	1.00	32.86	B
ATOM	3095	C	TYR	B	89	67.212	72.242	29.176	1.00	25.88	B
ATOM	3096	O	TYR	B	89	66.333	71.400	29.025	1.00	25.96	B
ATOM	3097	N	ARG	B	90	67.015	73.405	29.790	1.00	25.05	B
ATOM	3098	CA	ARG	B	90	65.732	73.778	30.386	1.00	21.94	B
ATOM	3099	CB	ARG	B	90	65.950	74.306	31.802	1.00	25.43	B
ATOM	3100	CG	ARG	B	90	66.836	73.368	32.650	1.00	35.30	B
ATOM	3101	CD	ARG	B	90	66.308	71.933	32.684	1.00	30.92	B
ATOM	3102	NE	ARG	B	90	65.162	71.857	33.578	1.00	38.77	B
ATOM	3103	CZ	ARG	B	90	64.577	70.721	33.950	1.00	43.50	B
ATOM	3104	NH1	ARG	B	90	65.038	69.562	33.500	1.00	42.19	B
ATOM	3105	NH2	ARG	B	90	63.529	70.750	34.771	1.00	39.16	B
ATOM	3106	C	ARG	B	90	65.001	74.823	29.580	1.00	26.84	B
ATOM	3107	O	ARG	B	90	65.540	75.372	28.606	1.00	21.63	B
ATOM	3108	N	HIS	B	91	63.767	75.095	29.999	1.00	24.57	B
ATOM	3109	CA	HIS	B	91	62.903	76.057	29.318	1.00	28.69	B
ATOM	3110	CB	HIS	B	91	61.570	76.143	30.062	1.00	26.54	B
ATOM	3111	CG	HIS	B	91	60.516	76.909	29.326	1.00	34.66	B
ATOM	3112	CD2	HIS	B	91	59.414	77.563	29.770	1.00	26.97	B
ATOM	3113	ND1	HIS	B	91	60.513	77.035	27.952	1.00	29.34	B
ATOM	3114	CE1	HIS	B	91	59.457	77.735	27.582	1.00	27.63	B
ATOM	3115	NE2	HIS	B	91	58.775	78.066	28.666	1.00	34.45	B
ATOM	3116	C	HIS	B	91	63.546	77.445	29.177	1.00	30.22	B
ATOM	3117	O	HIS	B	91	63.937	78.069	30.161	1.00	23.98	B
ATOM	3118	N	GLY	B	92	63.663	77.915	27.941	1.00	26.25	B
ATOM	3119	CA	GLY	B	92	64.260	79.209	27.702	1.00	20.48	B
ATOM	3120	C	GLY	B	92	65.752	79.118	27.458	1.00	24.40	B
ATOM	3121	O	GLY	B	92	66.310	80.102	27.019	1.00	24.34	B
ATOM	3122	N	ASP	B	93	66.407	77.974	27.724	1.00	20.35	B
ATOM	3123	CA	ASP	B	93	67.857	77.884	27.472	1.00	19.73	B
ATOM	3124	CB	ASP	B	93	68.487	76.575	27.992	1.00	23.61	B
ATOM	3125	CG	ASP	B	93	68.579	76.504	29.504	1.00	20.60	B
ATOM	3126	OD1	ASP	B	93	68.336	77.522	30.167	1.00	23.89	B
ATOM	3127	OD2	ASP	B	93	68.884	75.401	30.020	1.00	25.06	B
ATOM	3128	C	ASP	B	93	68.138	77.911	25.981	1.00	25.02	B
ATOM	3129	O	ASP	B	93	67.362	77.415	25.170	1.00	24.06	B
ATOM	3130	N	SER	B	94	69.298	78.422	25.625	1.00	21.77	B
ATOM	3131	CA	SER	B	94	69.641	78.511	24.229	1.00	27.05	B

ATOM	3132	CB	SER	B	94	69.779	79.972	23.834	1.00	28.57	B
ATOM	3133	OG	SER	B	94	70.417	80.035	22.587	1.00	38.84	B
ATOM	3134	C	SER	B	94	70.935	77.815	23.908	1.00	25.71	B
ATOM	3135	O	SER	B	94	71.833	77.727	24.753	1.00	26.52	B
ATOM	3136	N	VAL	B	95	71.051	77.331	22.678	1.00	27.36	B
ATOM	3137	CA	VAL	B	95	72.291	76.689	22.245	1.00	26.56	B
ATOM	3138	CB	VAL	B	95	72.096	75.178	22.088	1.00	26.82	B
ATOM	3139	CG1	VAL	B	95	73.282	74.581	21.344	1.00	34.06	B
ATOM	3140	CG2	VAL	B	95	71.908	74.549	23.460	1.00	30.69	B
ATOM	3141	C	VAL	B	95	72.729	77.273	20.908	1.00	30.07	B
ATOM	3142	O	VAL	B	95	71.903	77.496	20.019	1.00	26.03	B
ATOM	3143	N	THR	B	96	74.026	77.526	20.758	1.00	27.23	B
ATOM	3144	CA	THR	B	96	74.540	78.058	19.503	1.00	23.14	B
ATOM	3145	CB	THR	B	96	75.242	79.419	19.687	1.00	32.77	B
ATOM	3146	OG1	THR	B	96	74.292	80.383	20.163	1.00	26.94	B
ATOM	3147	CG2	THR	B	96	75.845	79.896	18.329	1.00	26.13	B
ATOM	3148	C	THR	B	96	75.550	77.071	18.915	1.00	33.62	B
ATOM	3149	O	THR	B	96	76.445	76.614	19.618	1.00	26.19	B
ATOM	3150	N	PHE	B	97	75.381	76.732	17.638	1.00	28.29	B
ATOM	3151	CA	PHE	B	97	76.249	75.788	16.922	1.00	27.82	B
ATOM	3152	CB	PHE	B	97	75.409	74.849	16.039	1.00	27.23	B
ATOM	3153	CG	PHE	B	97	74.598	73.858	16.796	1.00	30.99	B
ATOM	3154	CD1	PHE	B	97	73.325	74.183	17.257	1.00	28.10	B
ATOM	3155	CD2	PHE	B	97	75.149	72.633	17.153	1.00	24.15	B
ATOM	3156	CE1	PHE	B	97	72.608	73.310	18.081	1.00	29.54	B
ATOM	3157	CE2	PHE	B	97	74.434	71.756	17.975	1.00	26.96	B
ATOM	3158	CZ	PHE	B	97	73.155	72.101	18.444	1.00	28.76	B
ATOM	3159	C	PHE	B	97	77.247	76.479	15.980	1.00	33.87	B
ATOM	3160	O	PHE	B	97	77.088	77.663	15.628	1.00	30.90	B
ATOM	3161	N	ALA	B	98	78.074	75.725	15.582	1.00	33.98	B
ATOM	3162	CA	ALA	B	98	79.066	76.152	14.574	1.00	34.14	B
ATOM	3163	CB	ALA	B	98	80.551	76.651	15.211	1.00	38.55	B
ATOM	3164	C	ALA	B	98	79.544	74.880	13.785	1.00	36.15	B
ATOM	3165	O	ALA	B	98	79.370	73.775	14.312	1.00	35.98	B
ATOM	3166	N	CYS	B	99	79.952	75.018	12.527	1.00	38.50	B
ATOM	3167	CA	CYS	B	99	80.066	73.843	11.711	1.00	39.15	B
ATOM	3168	C	CYS	B	99	81.747	73.512	11.779	1.00	36.00	B
ATOM	3169	O	CYS	B	99	82.573	74.408	11.865	1.00	32.17	B
ATOM	3170	CB	CYS	B	99	79.901	74.086	10.251	1.00	42.12	B
ATOM	3171	SG	CYS	B	99	78.108	74.162	9.949	1.00	40.52	B
ATOM	3172	N	LYS	B	100	82.089	72.229	11.749	1.00	35.70	B
ATOM	3173	CA	LYS	B	100	83.498	71.842	11.770	1.00	40.35	B
ATOM	3174	CB	LYS	B	100	83.632	70.319	11.848	1.00	43.13	B
ATOM	3175	CG	LYS	B	100	83.185	69.707	13.148	1.00	38.59	B
ATOM	3176	CD	LYS	B	100	82.771	68.263	12.966	1.00	44.87	B
ATOM	3177	CE	LYS	B	100	82.689	67.562	14.314	1.00	48.06	B
ATOM	3178	NZ	LYS	B	100	82.353	66.122	14.196	1.00	53.59	B
ATOM	3179	C	LYS	B	100	84.190	72.329	10.482	1.00	45.56	B
ATOM	3180	O	LYS	B	100	83.532	72.770	9.525	1.00	42.57	B
ATOM	3181	N	THR	B	101	85.519	72.239	10.456	1.00	47.39	B
ATOM	3182	CA	THR	B	101	86.286	72.651	9.282	1.00	48.55	B
ATOM	3183	CB	THR	B	101	87.794	72.408	9.497	1.00	48.03	B
ATOM	3184	OG1	THR	B	101	88.281	73.285	10.521	1.00	47.14	B
ATOM	3185	CG2	THR	B	101	88.557	72.683	8.212	1.00	51.80	B
ATOM	3186	C	THR	B	101	85.816	71.876	8.042	1.00	47.72	B

ATOM	3187	O	THR	B	101	85.523	70.681	8.127	1.00	43.56	B
ATOM	3188	N	ASN	B	102	85.747	72.555	6.901	1.00	47.11	B
ATOM	3189	CA	ASN	B	102	85.294	71.943	5.647	1.00	48.36	B
ATOM	3190	CB	ASN	B	102	85.961	70.594	5.375	1.00	53.67	B
ATOM	3191	CG	ASN	B	102	87.461	70.703	5.219	1.00	58.65	B
ATOM	3192	OD1	ASN	B	102	87.980	71.763	4.856	1.00	59.24	B
ATOM	3193	ND2	ASN	B	102	88.171	69.599	5.484	1.00	61.19	B
ATOM	3194	C	ASN	B	102	83.797	71.728	5.632	1.00	49.36	B
ATOM	3195	O	ASN	B	102	83.284	70.965	4.814	1.00	51.85	B
ATOM	3196	N	PHE	B	103	83.097	72.378	6.555	1.00	48.85	B
ATOM	3197	CA	PHE	B	103	81.641	72.294	6.617	1.00	44.54	B
ATOM	3198	CB	PHE	B	103	81.179	71.539	7.855	1.00	44.01	B
ATOM	3199	CG	PHE	B	103	81.335	70.067	7.740	1.00	45.42	B
ATOM	3200	CD1	PHE	B	103	82.554	69.461	8.037	1.00	47.36	B
ATOM	3201	CD2	PHE	B	103	80.270	69.274	7.323	1.00	44.68	B
ATOM	3202	CE1	PHE	B	103	82.715	68.064	7.921	1.00	44.91	B
ATOM	3203	CE2	PHE	B	103	80.413	67.883	7.202	1.00	46.13	B
ATOM	3204	CZ	PHE	B	103	81.638	67.276	7.503	1.00	44.51	B
ATOM	3205	C	PHE	B	103	81.103	73.700	6.663	1.00	43.79	B
ATOM	3206	O	PHE	B	103	81.736	74.577	7.239	1.00	41.42	B
ATOM	3207	N	SER	B	104	79.939	73.908	6.052	1.00	46.45	B
ATOM	3208	CA	SER	B	104	79.306	75.216	6.007	1.00	47.47	B
ATOM	3209	CB	SER	B	104	79.176	75.706	4.570	1.00	53.61	B
ATOM	3210	OG	SER	B	104	77.886	75.379	4.057	1.00	61.85	B
ATOM	3211	C	SER	B	104	77.921	75.051	6.596	1.00	46.27	B
ATOM	3212	O	SER	B	104	77.285	74.007	6.425	1.00	46.36	B
ATOM	3213	N	MET	B	105	77.435	76.089	7.269	1.00	47.80	B
ATOM	3214	CA	MET	B	105	76.129	75.998	7.913	1.00	50.16	B
ATOM	3215	CB	MET	B	105	76.114	76.848	9.184	1.00	42.24	B
ATOM	3216	CG	MET	B	105	74.783	76.829	9.931	1.00	39.50	B
ATOM	3217	SD	MET	B	105	74.951	77.585	11.559	1.00	31.98	B
ATOM	3218	CE	MET	B	105	76.153	76.456	12.300	1.00	32.14	B
ATOM	3219	C	MET	B	105	74.948	76.398	7.046	1.00	52.75	B
ATOM	3220	O	MET	B	105	75.066	77.234	6.147	1.00	52.67	B
ATOM	3221	N	ASN	B	106	73.807	75.787	7.343	1.00	57.15	B
ATOM	3222	CA	ASN	B	106	72.560	76.072	6.664	1.00	56.25	B
ATOM	3223	CB	ASN	B	106	72.186	74.950	5.722	1.00	63.78	B
ATOM	3224	CG	ASN	B	106	72.679	75.210	4.332	1.00	72.25	B
ATOM	3225	OD1	ASN	B	106	72.787	76.372	3.916	1.00	78.63	B
ATOM	3226	ND2	ASN	B	106	72.995	74.141	3.597	1.00	74.20	B
ATOM	3227	C	ASN	B	106	71.504	76.200	7.727	1.00	54.17	B
ATOM	3228	O	ASN	B	106	71.303	75.277	8.508	1.00	56.24	B
ATOM	3229	N	GLY	B	107	70.833	77.342	7.762	1.00	50.67	B
ATOM	3230	CA	GLY	B	107	69.805	77.552	8.763	1.00	44.02	B
ATOM	3231	C	GLY	B	107	70.334	78.414	9.886	1.00	42.66	B
ATOM	3232	O	GLY	B	107	71.478	78.864	9.854	1.00	41.68	B
ATOM	3233	N	ASN	B	108	69.500	78.646	10.889	1.00	46.24	B
ATOM	3234	CA	ASN	B	108	69.878	79.464	12.032	1.00	47.08	B
ATOM	3235	CB	ASN	B	108	68.613	79.910	12.751	1.00	55.35	B
ATOM	3236	CG	ASN	B	108	67.793	80.851	11.903	1.00	63.30	B
ATOM	3237	OD1	ASN	B	108	68.164	82.013	11.722	1.00	67.44	B
ATOM	3238	ND2	ASN	B	108	66.691	80.352	11.346	1.00	68.11	B
ATOM	3239	C	ASN	B	108	70.808	78.723	12.981	1.00	39.04	B
ATOM	3240	O	ASN	B	108	70.560	77.577	13.347	1.00	33.47	B
ATOM	3241	N	LYS	B	109	71.858	79.406	13.402	1.00	34.53	B

ATOM	3242	CA	LYS	B	109	72.859	78.806	14.280	1.00	35.55	B
ATOM	3243	CB	LYS	B	109	74.138	79.632	14.217	1.00	35.53	B
ATOM	3244	CG	LYS	B	109	73.909	81.037	14.698	1.00	37.21	B
ATOM	3245	CD	LYS	B	109	75.176	81.691	15.171	1.00	43.67	B
ATOM	3246	CE	LYS	B	109	74.913	83.141	15.501	1.00	53.84	B
ATOM	3247	NZ	LYS	B	109	76.079	83.848	16.124	1.00	67.33	B
ATOM	3248	C	LYS	B	109	72.456	78.639	15.753	1.00	33.59	B
ATOM	3249	O	LYS	B	109	73.116	77.900	16.490	1.00	32.99	B
ATOM	3250	N	SER	B	110	71.409	79.337	16.198	1.00	29.02	B
ATOM	3251	CA	SER	B	110	70.972	79.239	17.597	1.00	31.62	B
ATOM	3252	CB	SER	B	110	71.068	80.588	18.298	1.00	28.39	B
ATOM	3253	OG	SER	B	110	72.395	81.073	18.276	1.00	35.28	B
ATOM	3254	C	SER	B	110	69.547	78.730	17.734	1.00	33.04	B
ATOM	3255	O	SER	B	110	68.665	79.049	16.935	1.00	28.18	B
ATOM	3256	N	VAL	B	111	69.336	77.927	18.761	1.00	32.94	B
ATOM	3257	CA	VAL	B	111	68.028	77.360	19.032	1.00	28.12	B
ATOM	3258	CB	VAL	B	111	67.998	75.911	18.507	1.00	34.53	B
ATOM	3259	CG1	VAL	B	111	69.117	75.074	19.143	1.00	27.59	B
ATOM	3260	CG2	VAL	B	111	66.694	75.304	18.785	1.00	41.47	B
ATOM	3261	C	VAL	B	111	67.729	77.488	20.539	1.00	26.65	B
ATOM	3262	O	VAL	B	111	68.631	77.621	21.359	1.00	27.71	B
ATOM	3263	N	TRP	B	112	66.447	77.496	20.866	1.00	26.33	B
ATOM	3264	CA	TRP	B	112	65.932	77.654	22.205	1.00	21.46	B
ATOM	3265	CB	TRP	B	112	65.023	78.895	22.287	1.00	27.43	B
ATOM	3266	CG	TRP	B	112	65.772	80.142	22.390	1.00	28.72	B
ATOM	3267	CD2	TRP	B	112	66.455	80.818	21.323	1.00	27.13	B
ATOM	3268	CE2	TRP	B	112	67.130	81.922	21.894	1.00	23.65	B
ATOM	3269	CE3	TRP	B	112	66.560	80.595	19.944	1.00	27.06	B
ATOM	3270	CD1	TRP	B	112	66.053	80.849	23.542	1.00	29.24	B
ATOM	3271	NE1	TRP	B	112	66.875	81.916	23.240	1.00	22.18	B
ATOM	3272	CZ2	TRP	B	112	67.896	82.804	21.132	1.00	24.55	B
ATOM	3273	CZ3	TRP	B	112	67.328	81.476	19.179	1.00	32.51	B
ATOM	3274	CH2	TRP	B	112	67.985	82.570	19.782	1.00	28.74	B
ATOM	3275	C	TRP	B	112	65.113	76.462	22.622	1.00	24.09	B
ATOM	3276	O	TRP	B	112	64.348	75.924	21.826	1.00	23.03	B
ATOM	3277	N	CYS	B	113	65.257	76.065	23.886	1.00	16.00	B
ATOM	3278	CA	CYS	B	113	64.507	74.942	24.421	1.00	22.66	B
ATOM	3279	C	CYS	B	113	63.090	75.442	24.775	1.00	27.37	B
ATOM	3280	O	CYS	B	113	62.892	76.248	25.700	1.00	23.71	B
ATOM	3281	CB	CYS	B	113	65.230	74.386	25.636	1.00	24.38	B
ATOM	3282	SG	CYS	B	113	64.295	73.084	26.474	1.00	25.70	B
ATOM	3283	N	GLN	B	114	62.105	74.973	24.014	1.00	22.77	B
ATOM	3284	CA	GLN	B	114	60.704	75.406	24.190	1.00	27.53	B
ATOM	3285	CB	GLN	B	114	59.993	75.312	22.852	1.00	23.87	B
ATOM	3286	CG	GLN	B	114	60.669	76.101	21.776	1.00	25.80	B
ATOM	3287	CD	GLN	B	114	59.934	75.957	20.455	1.00	34.33	B
ATOM	3288	OE1	GLN	B	114	59.540	74.850	20.084	1.00	40.82	B
ATOM	3289	NE2	GLN	B	114	59.749	77.062	19.744	1.00	28.51	B
ATOM	3290	C	GLN	B	114	59.918	74.632	25.242	1.00	24.17	B
ATOM	3291	O	GLN	B	114	60.324	73.557	25.638	1.00	24.70	B
ATOM	3292	N	ALA	B	115	58.806	75.187	25.704	1.00	28.17	B
ATOM	3293	CA	ALA	B	115	57.984	74.520	26.720	1.00	32.79	B
ATOM	3294	CB	ALA	B	115	56.769	75.392	27.068	1.00	30.00	B
ATOM	3295	C	ALA	B	115	57.523	73.107	26.316	1.00	34.03	B
ATOM	3296	O	ALA	B	115	57.338	72.237	27.170	1.00	33.21	B

ATOM	3297	N	ASN	B	115	57.343	72.881	25.020	1.00 36.70	B
ATOM	3298	CA	ASN	B	116	56.913	71.573	24.526	1.00 38.02	B
ATOM	3299	CB	ASN	B	116	56.230	71.728	23.168	1.00 34.90	B
ATOM	3300	CG	ASN	B	116	57.198	72.144	22.087	1.00 33.42	B
ATOM	3301	OD1	ASN	B	116	58.359	72.454	22.364	1.00 28.93	B
ATOM	3302	ND2	ASN	B	116	56.728	72.167	20.853	1.00 30.98	B
ATOM	3303	C	ASN	B	116	58.104	70.608	24.392	1.00 34.77	B
ATOM	3304	O	ASN	B	116	58.017	69.612	23.695	1.00 37.54	B
ATOM	3305	N	ASN	B	117	59.219	70.937	25.044	1.00 36.92	B
ATOM	3306	CA	ASN	B	117	60.425	70.094	25.072	1.00 31.01	B
ATOM	3307	CB	ASN	B	117	60.095	68.728	25.699	1.00 35.95	B
ATOM	3308	CG	ASN	B	117	59.327	68.855	27.022	1.00 41.69	B
ATOM	3309	OD1	ASN	B	117	58.165	68.448	27.116	1.00 48.82	B
ATOM	3310	ND2	ASN	B	117	59.966	69.428	28.041	1.00 38.48	B
ATOM	3311	C	ASN	B	117	61.155	69.913	23.753	1.00 35.04	B
ATOM	3312	O	ASN	B	117	61.989	69.010	23.584	1.00 30.97	B
ATOM	3313	N	MET	B	118	60.877	70.804	22.814	1.00 32.90	B
ATOM	3314	CA	MET	B	118	61.544	70.747	21.539	1.00 30.69	B
ATOM	3315	CB	MET	B	118	60.533	70.486	20.426	1.00 39.19	B
ATOM	3316	CG	MET	B	118	60.143	69.004	20.284	1.00 45.35	B
ATOM	3317	SD	MET	B	118	58.844	68.904	19.065	1.00 61.98	B
ATOM	3318	CE	MET	B	118	57.379	68.930	20.152	1.00 59.12	B
ATOM	3319	C	MET	B	118	62.299	72.033	21.290	1.00 32.74	B
ATOM	3320	O	MET	B	118	61.958	73.093	21.820	1.00 31.41	B
ATOM	3321	N	TRP	B	119	63.322	71.913	20.460	1.00 30.27	B
ATOM	3322	CA	TRP	B	119	64.197	73.007	20.122	1.00 32.04	B
ATOM	3323	CB	TRP	B	119	65.519	72.477	19.556	1.00 29.45	B
ATOM	3324	CG	TRP	B	119	66.377	71.888	20.618	1.00 34.08	B
ATOM	3325	CD2	TRP	B	119	67.091	72.613	21.638	1.00 29.55	B
ATOM	3326	CE2	TRP	B	119	67.641	71.653	22.514	1.00 32.16	B
ATOM	3327	CE3	TRP	B	119	67.309	73.974	21.891	1.00 27.61	B
ATOM	3328	CD1	TRP	B	119	66.533	70.563	20.907	1.00 27.66	B
ATOM	3329	NE1	TRP	B	119	67.287	70.419	22.045	1.00 29.97	B
ATOM	3330	CZ2	TRP	B	119	68.401	72.018	23.634	1.00 33.69	B
ATOM	3331	CZ3	TRP	B	119	68.067	74.333	23.002	1.00 28.67	B
ATOM	3332	CH2	TRP	B	119	68.603	73.356	23.860	1.00 29.17	B
ATOM	3333	C	TRP	B	119	63.672	74.059	19.188	1.00 35.37	B
ATOM	3334	O	TRP	B	119	62.946	73.750	18.264	1.00 34.01	B
ATOM	3335	N	GLY	B	120	64.129	75.279	19.507	1.00 44.82	B
ATOM	3336	CA	GLY	B	120	63.928	76.577	18.868	1.00 40.39	B
ATOM	3337	C	GLY	B	120	62.736	76.818	18.037	1.00 45.27	B
ATOM	3338	O	GLY	B	120	61.922	75.920	17.884	1.00 54.52	B
ATOM	3339	N	PRO	B	121	62.570	78.049	17.525	1.00 39.72	B
ATOM	3340	CD	PRO	B	121	63.331	79.268	17.805	1.00 34.64	B
ATOM	3341	CA	PRO	B	121	61.411	78.339	16.678	1.00 40.69	B
ATOM	3342	CB	PRO	B	121	61.355	79.869	16.674	1.00 38.54	B
ATOM	3343	CG	PRO	B	121	62.781	80.221	16.775	1.00 38.11	B
ATOM	3344	C	PRO	B	121	61.717	77.733	15.294	1.00 38.17	B
ATOM	3345	O	PRO	B	121	60.817	77.305	14.591	1.00 40.16	B
ATOM	3346	N	THR	B	122	62.994	77.693	14.930	1.00 33.84	B
ATOM	3347	CA	THR	B	122	63.424	77.113	13.660	1.00 38.91	B
ATOM	3348	CB	THR	B	122	64.548	77.939	12.988	1.00 42.26	B
ATOM	3349	OG1	THR	B	122	65.803	77.671	13.634	1.00 39.47	B
ATOM	3350	CG2	THR	B	122	64.259	79.431	13.106	1.00 40.58	B
ATOM	3351	C	THR	B	122	63.968	75.708	13.874	1.00 40.61	B

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ATOM   3352  O   THR B 122      64.163  75.266  14.999  1.00 43.52      B
ATOM   3353  N   ARG B 123      64.220  75.005  12.784  1.00 42.70      B
ATOM   3354  CA  ARG B 123      64.762  73.656  12.870  1.00 46.43      B
ATOM   3355  CB  ARG B 123      64.505  72.912  11.549  1.00 48.19      B
ATOM   3356  CG  ARG B 123      64.849  71.433  11.600  1.00 63.34      B
ATOM   3357  CD  ARG B 123      64.109  70.638  10.517  1.00 71.72      B
ATOM   3358  NE  ARG B 123      62.664  70.564  10.762  1.00 75.72      B
ATOM   3359  CZ  ARG B 123      61.734  70.934   9.881  1.00 77.53      B
ATOM   3360  NH1 ARG B 123      62.096  71.410   8.690  1.00 78.13      B
ATOM   3361  NH2 ARG B 123      60.444  70.820  10.184  1.00 75.29      B
ATOM   3362  C   ARG B 123      66.270  73.774  13.141  1.00 36.14      B
ATOM   3363  O   ARG B 123      66.861  74.816  12.880  1.00 34.06      B
ATOM   3364  N   LEU B 124      66.888  72.714  13.659  1.00 36.62      B
ATOM   3365  CA  LEU B 124      68.326  72.743  13.939  1.00 35.68      B
ATOM   3366  CB  LEU B 124      68.818  71.410  14.509  1.00 37.22      B
ATOM   3367  CG  LEU B 124      68.399  71.019  15.933  1.00 38.68      B
ATOM   3368  CD1 LEU B 124      69.008  69.670  16.342  1.00 37.12      B
ATOM   3369  CD2 LEU B 124      68.860  72.097  16.874  1.00 34.15      B
ATOM   3370  C   LEU B 124      69.081  73.029  12.656  1.00 37.07      B
ATOM   3371  O   LEU B 124      68.701  72.584  11.583  1.00 35.87      B
ATOM   3372  N   PRO B 125      70.168  73.787  12.750  1.00 40.36      B
ATOM   3373  CD  PRO B 125      70.832  74.306  13.962  1.00 38.05      B
ATOM   3374  CA  PRO B 125      70.933  74.085  11.538  1.00 35.47      B
ATOM   3375  CB  PRO B 125      71.993  75.069  12.029  1.00 35.51      B
ATOM   3376  CG  PRO B 125      72.224  74.641  13.460  1.00 35.57      B
ATOM   3377  C   PRO B 125      71.535  72.794  11.002  1.00 40.45      B
ATOM   3378  O   PRO B 125      71.432  71.739  11.640  1.00 33.92      B
ATOM   3379  N   THR B 126      72.131  72.867   9.814  1.00 41.58      B
ATOM   3380  CA  THR B 126      72.765  71.704   9.217  1.00 41.03      B
ATOM   3381  CB  THR B 126      71.929  71.137   8.006  1.00 42.99      B
ATOM   3382  OG1 THR B 126      71.625  72.182   7.075  1.00 45.10      B
ATOM   3383  CG2 THR B 126      70.628  70.529   8.503  1.00 40.83      B
ATOM   3384  C   THR B 126      74.157  72.116   8.777  1.00 41.16      B
ATOM   3385  O   THR B 126      74.415  73.299   8.544  1.00 40.35      B
ATOM   3386  N   CYS B 127      75.074  71.158   8.716  1.00 42.86      B
ATOM   3387  CA  CYS B 127      76.433  71.468   8.279  1.00 48.44      B
ATOM   3388  C   CYS B 127      76.774  70.561   7.098  1.00 53.76      B
ATOM   3389  O   CYS B 127      76.711  69.336   7.219  1.00 55.59      B
ATOM   3390  CB  CYS B 127      77.440  71.249   9.422  1.00 49.29      B
ATOM   3391  SG  CYS B 127      77.365  72.471  10.779  1.00 41.21      B
ATOM   3392  N   VAL B 128      77.117  71.159   5.960  1.00 52.99      B
ATOM   3393  CA  VAL B 128      77.466  70.386   4.764  1.00 58.11      B
ATOM   3394  CB  VAL B 128      76.479  70.674   3.612  1.00 60.17      B
ATOM   3395  CG1 VAL B 128      76.356  72.179   3.395  1.00 59.61      B
ATOM   3396  CG2 VAL B 128      76.974  70.005   2.322  1.00 62.78      B
ATOM   3397  C   VAL B 128      78.881  70.738   4.290  1.00 55.96      B
ATOM   3398  O   VAL B 128      79.307  71.875   4.427  1.00 56.76      B
ATOM   3399  N   SER B 129      79.604  69.763   3.747  1.00 56.88      B
ATOM   3400  CA  SER B 129      80.976  69.974   3.241  1.00 63.04      B
ATOM   3401  CB  SER B 129      81.489  68.685   2.616  1.00 64.42      B
ATOM   3402  OG  SER B 129      80.566  68.249   1.633  1.00 74.77      B
ATOM   3403  C   SER B 129      81.061  71.092   2.194  1.00 60.01      B
ATOM   3404  O   SER B 129      82.054  71.856   2.166  1.00 59.63      B
ATOM   3405  OXT SER B 129      80.121  71.165   1.381  1.00 61.43      B
ATOM   3406  CB  ALA C   1      51.630  81.929   2.879  1.00 35.79      C
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ATOM	3407	C	ALA	C	1	50.853	84.288	2.366	1.00	35.46	C
ATOM	3408	O	ALA	C	1	50.053	85.212	2.282	1.00	40.99	C
ATOM	3409	N	ALA	C	1	49.558	82.473	1.552	1.00	39.80	C
ATOM	3410	CA	ALA	C	1	50.332	82.883	2.708	1.00	38.04	C
ATOM	3411	N	ILE	C	2	52.138	84.436	2.113	1.00	25.56	C
ATOM	3412	CA	ILE	C	2	52.684	85.736	1.810	1.00	32.00	C
ATOM	3413	CB	ILE	C	2	53.982	85.933	2.591	1.00	24.33	C
ATOM	3414	CG2	ILE	C	2	54.794	87.063	1.974	1.00	24.84	C
ATOM	3415	CG1	ILE	C	2	53.647	86.140	4.085	1.00	31.72	C
ATOM	3416	CD1	ILE	C	2	54.375	86.286	5.004	1.00	28.23	C
ATOM	3417	C	ILE	C	2	52.955	85.930	0.331	1.00	29.98	C
ATOM	3418	O	ILE	C	2	53.280	84.966	-0.364	1.00	24.28	C
ATOM	3419	N	SER	C	3	52.816	87.164	-0.156	1.00	25.13	C
ATOM	3420	CA	SER	C	3	53.130	87.453	-1.564	1.00	24.56	C
ATOM	3421	CB	SER	C	3	51.848	87.773	-2.360	1.00	23.32	C
ATOM	3422	OG	SER	C	3	51.206	88.949	-1.866	1.00	28.18	C
ATOM	3423	C	SER	C	3	54.111	88.630	-1.651	1.00	28.79	C
ATOM	3424	O	SER	C	3	54.240	89.413	-0.703	1.00	25.00	C
ATOM	3425	N	CYS	C	4	54.834	88.720	-2.766	1.00	24.82	C
ATOM	3426	CA	CYS	C	4	55.760	89.824	-3.003	1.00	23.87	C
ATOM	3427	C	CYS	C	4	55.114	90.751	-4.020	1.00	26.63	C
ATOM	3428	O	CYS	C	4	54.488	90.277	-4.974	1.00	24.86	C
ATOM	3429	CB	CYS	C	4	57.075	89.341	-3.595	1.00	26.41	C
ATOM	3430	SG	CYS	C	4	58.182	88.516	-2.412	1.00	26.19	C
ATOM	3431	N	GLY	C	5	55.270	92.056	-3.843	1.00	25.01	C
ATOM	3432	CA	GLY	C	5	54.697	93.002	-4.800	1.00	23.78	C
ATOM	3433	C	GLY	C	5	55.467	93.100	-6.115	1.00	33.19	C
ATOM	3434	O	GLY	C	5	56.444	92.346	-6.350	1.00	24.73	C
ATOM	3435	N	SER	C	6	55.020	94.068	-6.975	1.00	24.24	C
ATOM	3436	CA	SER	C	6	55.654	94.257	-8.285	1.00	31.29	C
ATOM	3437	CB	SER	C	6	54.994	95.528	-8.834	1.00	28.12	C
ATOM	3438	OG	SER	C	6	53.739	95.485	-9.097	1.00	30.57	C
ATOM	3439	C	SER	C	6	57.187	94.422	-8.106	1.00	28.51	C
ATOM	3440	O	SER	C	6	57.681	95.162	-7.262	1.00	27.78	C
ATOM	3441	N	PRO	C	7	57.931	93.562	-8.849	1.00	24.89	C
ATOM	3442	CD	PRO	C	7	57.432	92.669	-9.919	1.00	29.34	C
ATOM	3443	CA	PRO	C	7	59.391	93.554	-8.765	1.00	29.21	C
ATOM	3444	CB	PRO	C	7	59.778	92.308	-9.570	1.00	30.50	C
ATOM	3445	CG	PRO	C	7	58.721	92.286	-10.660	1.00	34.19	C
ATOM	3446	C	PRO	C	7	60.066	94.829	-9.286	1.00	25.82	C
ATOM	3447	O	PRO	C	7	59.490	95.586	-10.054	1.00	30.82	C
ATOM	3448	N	PRO	C	8	61.312	95.071	-8.879	1.00	25.55	C
ATOM	3449	CD	PRO	C	8	62.239	94.221	-8.107	1.00	22.99	C
ATOM	3450	CA	PRO	C	8	61.972	96.293	-9.360	1.00	27.11	C
ATOM	3451	CB	PRO	C	8	63.315	96.292	-8.613	1.00	23.33	C
ATOM	3452	CG	PRO	C	8	63.116	95.255	-7.464	1.00	30.29	C
ATOM	3453	C	PRO	C	8	62.162	96.260	-10.877	1.00	27.57	C
ATOM	3454	O	PRO	C	8	62.478	95.206	-11.457	1.00	27.35	C
ATOM	3455	N	PRO	C	9	61.945	97.401	-11.553	1.00	28.23	C
ATOM	3456	CD	PRO	C	9	61.527	98.718	-11.049	1.00	30.53	C
ATOM	3457	CA	PRO	C	9	62.116	97.415	-13.009	1.00	29.41	C
ATOM	3458	CB	PRO	C	9	61.430	98.714	-13.417	1.00	30.12	C
ATOM	3459	CG	PRO	C	9	61.742	99.607	-12.272	1.00	31.67	C
ATOM	3460	C	PRO	C	9	63.607	97.389	-13.404	1.00	37.14	C
ATOM	3461	O	PRO	C	9	64.487	97.661	-12.572	1.00	30.31	C

ATOM	3462	N	ILE	C	10	63.883	97.070	-14.669	1.00	30.28	C
ATOM	3463	CA	ILE	C	10	65.252	97.015	-15.166	1.00	29.72	C
ATOM	3464	CB	ILE	C	10	65.704	95.533	-15.351	1.00	30.40	C
ATOM	3465	CG2	ILE	C	10	64.708	94.766	-16.273	1.00	30.23	C
ATOM	3466	CG1	ILE	C	10	67.121	95.474	-15.931	1.00	28.32	C
ATOM	3467	CD1	ILE	C	10	67.729	94.058	-15.907	1.00	27.53	C
ATOM	3468	C	ILE	C	10	65.380	97.792	-16.488	1.00	36.89	C
ATOM	3469	O	ILE	C	10	64.732	97.472	-17.491	1.00	34.25	C
ATOM	3470	N	LEU	C	11	66.219	98.822	-16.483	1.00	38.68	C
ATOM	3471	CA	LEU	C	11	66.436	99.629	-17.678	1.00	36.69	C
ATOM	3472	CB	LEU	C	11	67.259	100.846	-17.320	1.00	40.95	C
ATOM	3473	CG	LEU	C	11	66.804	102.189	-17.855	1.00	45.07	C
ATOM	3474	CD1	LEU	C	11	65.484	102.575	-17.199	1.00	43.54	C
ATOM	3475	CD2	LEU	C	11	67.875	103.215	-17.565	1.00	43.98	C
ATOM	3476	C	LEU	C	11	67.176	98.837	-18.758	1.00	39.52	C
ATOM	3477	O	LEU	C	11	68.193	98.204	-18.475	1.00	37.78	C
ATOM	3478	N	ASN	C	12	66.636	98.899	-19.988	1.00	30.25	C
ATOM	3479	CA	ASN	C	12	67.284	98.227	-21.121	1.00	28.03	C
ATOM	3480	CB	ASN	C	12	68.705	98.746	-21.351	1.00	38.34	C
ATOM	3481	CG	ASN	C	12	68.739	100.231	-21.653	1.00	42.68	C
ATOM	3482	OD1	ASN	C	12	69.139	101.036	-20.813	1.00	47.15	C
ATOM	3483	ND2	ASN	C	12	68.318	100.596	-22.859	1.00	44.31	C
ATOM	3484	C	ASN	C	12	67.294	96.721	-20.910	1.00	36.66	C
ATOM	3485	O	ASN	C	12	68.253	96.075	-21.417	1.00	38.52	C
ATOM	3486	N	GLY	C	13	66.330	96.216	-20.179	1.00	37.43	C
ATOM	3487	CA	GLY	C	13	66.219	94.783	-19.993	1.00	37.37	C
ATOM	3488	C	GLY	C	13	64.776	94.380	-19.800	1.00	34.87	C
ATOM	3489	O	GLY	C	13	63.859	95.180	-19.928	1.00	37.34	C
ATOM	3490	N	ARG	C	14	64.557	93.119	-19.493	1.00	35.59	C
ATOM	3491	CA	ARG	C	14	63.201	92.681	-19.259	1.00	36.84	C
ATOM	3492	CB	ARG	C	14	62.562	92.191	-20.558	1.00	41.62	C
ATOM	3493	CG	ARG	C	14	63.333	91.087	-21.221	1.00	51.45	C
ATOM	3494	CD	ARG	C	14	63.739	91.505	-22.634	1.00	65.10	C
ATOM	3495	NE	ARG	C	14	64.692	92.626	-22.649	1.00	73.47	C
ATOM	3496	CZ	ARG	C	14	64.669	93.630	-23.528	1.00	76.84	C
ATOM	3497	NH1	ARG	C	14	63.736	93.667	-24.477	1.00	76.76	C
ATOM	3498	NH2	ARG	C	14	65.576	94.600	-23.457	1.00	76.89	C
ATOM	3499	C	ARG	C	14	63.179	91.573	-18.224	1.00	34.90	C
ATOM	3500	O	ARG	C	14	64.211	90.974	-17.875	1.00	30.74	C
ATOM	3501	N	ILE	C	15	61.985	91.308	-17.725	1.00	32.52	C
ATOM	3502	CA	ILE	C	15	61.809	90.274	-16.740	1.00	35.90	C
ATOM	3503	CB	ILE	C	15	61.048	90.814	-15.525	1.00	31.54	C
ATOM	3504	CG2	ILE	C	15	60.749	89.677	-14.553	1.00	25.41	C
ATOM	3505	CG1	ILE	C	15	61.862	91.952	-14.893	1.00	30.46	C
ATOM	3506	CD1	ILE	C	15	61.086	92.836	-13.959	1.00	28.46	C
ATOM	3507	C	ILE	C	15	61.013	89.156	-17.357	1.00	39.71	C
ATOM	3508	O	ILE	C	15	60.004	88.403	-18.022	1.00	39.51	C
ATOM	3509	N	SER	C	16	61.469	87.930	-17.136	1.00	39.22	C
ATOM	3510	CA	SER	C	16	60.762	86.750	-17.623	1.00	50.26	C
ATOM	3511	CB	SER	C	16	61.410	85.472	-17.077	1.00	53.90	C
ATOM	3512	OG	SER	C	16	61.213	85.384	-15.655	1.00	59.12	C
ATOM	3513	C	SER	C	16	59.326	86.801	-17.091	1.00	50.15	C
ATOM	3514	O	SER	C	16	59.097	87.096	-15.911	1.00	46.35	C
ATOM	3515	N	TYR	C	17	58.377	86.475	-17.961	1.00	54.91	C
ATOM	3516	CA	TYR	C	17	56.951	86.453	-17.629	1.00	50.96	C

ATOM	3517	CB	TYR	C	17	56.154	85.806	-18.765	1.00	56.78	C
ATOM	3518	CG	TYR	C	17	54.665	86.055	-18.678	1.00	58.05	C
ATOM	3519	CD1	TYR	C	17	54.109	87.224	-19.209	1.00	59.99	C
ATOM	3520	CE1	TYR	C	17	52.751	87.504	-19.071	1.00	61.22	C
ATOM	3521	CD2	TYR	C	17	53.822	85.163	-18.004	1.00	55.94	C
ATOM	3522	CE2	TYR	C	17	52.457	85.438	-17.854	1.00	58.29	C
ATOM	3523	CZ	TYR	C	17	51.926	86.620	-18.395	1.00	61.48	C
ATOM	3524	OH	TYR	C	17	50.577	86.917	-18.272	1.00	63.66	C
ATOM	3525	C	TYR	C	17	56.708	85.652	-16.360	1.00	49.21	C
ATOM	3526	O	TYR	C	17	57.228	84.555	-16.189	1.00	51.47	C
ATOM	3527	N	TYR	C	18	55.921	86.212	-15.459	1.00	49.68	C
ATOM	3528	CA	TYR	C	18	55.600	85.528	-14.218	1.00	46.63	C
ATOM	3529	CB	TYR	C	18	56.361	86.154	-13.033	1.00	42.78	C
ATOM	3530	CG	TYR	C	18	56.242	87.663	-12.969	1.00	35.46	C
ATOM	3531	CD1	TYR	C	18	57.129	88.488	-13.678	1.00	36.33	C
ATOM	3532	CE1	TYR	C	18	56.996	89.880	-13.663	1.00	33.08	C
ATOM	3533	CD2	TYR	C	18	55.220	88.270	-12.243	1.00	29.58	C
ATOM	3534	CE2	TYR	C	18	55.083	89.665	-12.218	1.00	29.35	C
ATOM	3535	CZ	TYR	C	18	55.968	90.465	-12.921	1.00	27.89	C
ATOM	3536	OH	TYR	C	18	55.863	91.850	-12.860	1.00	32.49	C
ATOM	3537	C	TYR	C	18	54.100	85.695	-14.022	1.00	43.03	C
ATOM	3538	O	TYR	C	18	53.496	86.659	-14.513	1.00	41.84	C
ATOM	3539	N	SER	C	19	53.496	84.758	-13.314	1.00	44.03	C
ATOM	3540	CA	SER	C	19	52.067	84.849	-13.068	1.00	49.05	C
ATOM	3541	CB	SER	C	19	51.430	83.455	-13.036	1.00	48.59	C
ATOM	3542	OG	SER	C	19	52.115	82.585	-12.147	1.00	50.14	C
ATOM	3543	C	SER	C	19	51.823	85.584	-11.749	1.00	50.35	C
ATOM	3544	O	SER	C	19	52.661	85.567	-10.839	1.00	46.39	C
ATOM	3545	N	THR	C	20	50.607	86.109	-11.537	1.00	52.04	C
ATOM	3546	CA	THR	C	20	50.099	86.977	-10.488	1.00	53.58	C
ATOM	3547	CB	THR	C	20	49.571	88.093	-11.054	1.00	55.84	C
ATOM	3548	OG1	THR	C	20	48.476	88.030	-11.940	1.00	60.69	C
ATOM	3549	CG2	THR	C	20	50.671	89.029	-11.802	1.00	52.60	C
ATOM	3550	C	THR	C	20	49.003	86.277	-9.703	1.00	56.21	C
ATOM	3551	O	THR	C	20	48.037	85.783	-10.339	1.00	59.04	C
ATOM	3552	N	PRO	C	21	49.034	86.244	-8.386	1.00	47.82	C
ATOM	3553	CD	PRO	C	21	48.004	85.901	-7.826	1.00	47.40	C
ATOM	3554	CA	PRO	C	21	50.027	86.916	-7.519	1.00	42.99	C
ATOM	3555	CB	PRO	C	21	49.335	86.932	-6.151	1.00	43.36	C
ATOM	3556	CG	PRO	C	21	48.022	86.266	-6.380	1.00	47.21	C
ATOM	3557	C	PRO	C	21	51.356	86.153	-7.464	1.00	39.76	C
ATOM	3558	O	PRO	C	21	51.481	85.058	-8.071	1.00	37.13	C
ATOM	3559	N	ILE	C	22	52.324	86.813	-6.805	1.00	33.73	C
ATOM	3560	CA	ILE	C	22	53.646	86.316	-6.676	1.00	31.36	C
ATOM	3561	CB	ILE	C	22	54.709	87.316	-6.985	1.00	33.33	C
ATOM	3562	CG2	ILE	C	22	56.125	86.572	-6.755	1.00	33.08	C
ATOM	3563	CG1	ILE	C	22	54.641	87.724	-8.423	1.00	24.06	C
ATOM	3564	CD1	ILE	C	22	55.565	88.878	-8.747	1.00	24.35	C
ATOM	3565	C	ILE	C	22	53.824	85.628	-5.269	1.00	34.54	C
ATOM	3566	O	ILE	C	22	53.977	86.348	-4.285	1.00	28.13	C
ATOM	3567	N	ALA	C	23	53.864	84.299	-5.155	1.00	28.78	C
ATOM	3568	CA	ALA	C	23	54.048	83.695	-3.836	1.00	30.59	C
ATOM	3569	CB	ALA	C	23	53.437	82.316	-3.834	1.00	31.70	C
ATOM	3570	C	ALA	C	23	55.517	83.599	-3.412	1.00	30.12	C
ATOM	3571	O	ALA	C	23	56.399	83.517	-4.266	1.00	25.80	C

ATOM	3572	N	VAL	C	24	55.784	83.613	-2.102	1.00	32.21	C
ATOM	3573	CA	VAL	C	24	57.165	83.456	-1.625	1.00	30.00	C
ATOM	3574	CB	VAL	C	24	57.272	83.290	-0.087	1.00	35.52	C
ATOM	3575	CG1	VAL	C	24	56.808	84.563	0.597	1.00	35.78	C
ATOM	3576	CG2	VAL	C	24	56.459	82.108	0.378	1.00	39.11	C
ATOM	3577	C	VAL	C	24	57.673	82.175	-2.253	1.00	31.34	C
ATOM	3578	O	VAL	C	24	56.918	81.231	-2.413	1.00	28.53	C
ATOM	3579	N	GLY	C	25	58.947	82.128	-2.603	1.00	30.39	C
ATOM	3580	CA	GLY	C	25	59.456	80.936	-3.249	1.00	32.92	C
ATOM	3581	C	GLY	C	25	59.526	81.119	-4.764	1.00	34.28	C
ATOM	3582	O	GLY	C	25	60.245	80.389	-5.443	1.00	37.66	C
ATOM	3583	N	THR	C	26	58.785	82.086	-5.296	1.00	25.38	C
ATOM	3584	CA	THR	C	26	58.791	82.337	-6.735	1.00	33.97	C
ATOM	3585	CB	THR	C	26	57.652	83.304	-7.169	1.00	27.23	C
ATOM	3586	OG1	THR	C	26	56.390	82.761	-6.784	1.00	35.09	C
ATOM	3587	CG2	THR	C	26	57.650	83.514	-8.696	1.00	27.35	C
ATOM	3588	C	THR	C	26	60.113	82.985	-7.132	1.00	35.06	C
ATOM	3589	O	THR	C	26	60.614	83.888	-6.441	1.00	32.34	C
ATOM	3590	N	VAL	C	27	60.662	82.523	-8.246	1.00	27.52	C
ATOM	3591	CA	VAL	C	27	61.914	83.046	-8.795	1.00	30.48	C
ATOM	3592	CB	VAL	C	27	62.901	81.912	-9.116	1.00	35.60	C
ATOM	3593	CG1	VAL	C	27	64.064	82.451	-9.936	1.00	34.59	C
ATOM	3594	CG2	VAL	C	27	63.398	81.269	-7.830	1.00	34.12	C
ATOM	3595	C	VAL	C	27	61.632	82.751	-10.114	1.00	32.83	C
ATOM	3596	O	VAL	C	27	60.908	83.216	-10.953	1.00	31.75	C
ATOM	3597	N	ILE	C	28	62.168	84.956	-10.310	1.00	31.95	C
ATOM	3598	CA	ILE	C	28	61.967	85.628	-11.600	1.00	25.76	C
ATOM	3599	CB	ILE	C	28	61.234	86.962	-11.482	1.00	25.19	C
ATOM	3600	CG2	ILE	C	28	59.782	86.710	-11.057	1.00	27.07	C
ATOM	3601	CG1	ILE	C	28	61.981	87.915	-10.539	1.00	20.91	C
ATOM	3602	CD1	ILE	C	28	61.363	89.345	-10.512	1.00	24.89	C
ATOM	3603	C	ILE	C	28	63.341	85.870	-12.187	1.00	29.97	C
ATOM	3604	O	ILE	C	28	64.341	85.934	-11.450	1.00	24.78	C
ATOM	3605	N	ARG	C	29	63.394	86.015	-13.505	1.00	31.68	C
ATOM	3606	CA	ARG	C	29	64.673	86.191	-14.185	1.00	33.25	C
ATOM	3607	CB	ARG	C	29	64.962	84.984	-15.093	1.00	43.21	C
ATOM	3608	CG	ARG	C	29	65.539	83.751	-14.395	1.00	55.79	C
ATOM	3609	CD	ARG	C	29	64.795	82.458	-14.794	1.00	63.30	C
ATOM	3610	NE	ARG	C	29	63.873	82.000	-13.745	1.00	66.73	C
ATOM	3611	CZ	ARG	C	29	62.570	81.762	-13.917	1.00	68.37	C
ATOM	3612	NH1	ARG	C	29	62.003	81.935	-15.119	1.00	66.91	C
ATOM	3613	NH2	ARG	C	29	61.831	81.353	-12.983	1.00	61.65	C
ATOM	3614	C	ARG	C	29	64.794	87.444	-15.020	1.00	30.28	C
ATOM	3615	O	ARG	C	29	63.956	87.732	-15.873	1.00	29.65	C
ATOM	3616	N	TYR	C	30	65.867	88.181	-14.778	1.00	32.96	C
ATOM	3617	CA	TYR	C	30	66.159	89.400	-15.527	1.00	31.51	C
ATOM	3618	CB	TYR	C	30	66.759	90.437	-14.590	1.00	27.74	C
ATOM	3619	CG	TYR	C	30	65.773	91.001	-13.617	1.00	23.76	C
ATOM	3620	CD1	TYR	C	30	65.257	90.224	-12.571	1.00	28.24	C
ATOM	3621	CE1	TYR	C	30	64.350	90.773	-11.631	1.00	28.16	C
ATOM	3622	CD2	TYR	C	30	65.360	92.327	-13.718	1.00	27.82	C
ATOM	3623	CE2	TYR	C	30	64.456	92.879	-12.793	1.00	28.53	C
ATOM	3624	CZ	TYR	C	30	63.971	92.097	-11.758	1.00	22.02	C
ATOM	3625	OH	TYR	C	30	63.160	92.703	-10.848	1.00	24.79	C
ATOM	3626	C	TYR	C	30	67.161	89.133	-16.641	1.00	25.91	C

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ATOM   3627  O   TYR C  30      68.007  88.254 -16.520  1.00 26.19      C
ATOM   3628  N   SER C  31      67.065  89.883 -17.731  1.00 28.15      C
ATOM   3629  CA  SER C  31      68.027  89.740 -18.811  1.00 28.99      C
ATOM   3630  CB  SER C  31      67.611  88.643 -19.795  1.00 25.70      C
ATOM   3631  OG  SER C  31      66.381  88.981 -20.380  1.00 32.01      C
ATOM   3632  C   SER C  31      68.124  91.082 -19.518  1.00 30.27      C
ATOM   3633  O   SER C  31      67.213  91.910 -19.437  1.00 31.07      C
ATOM   3634  N   CYS C  32      69.238  91.304 -20.192  1.00 27.74      C
ATOM   3635  CA  CYS C  32      69.457  92.558 -20.890  1.00 32.43      C
ATOM   3636  C   CYS C  32      69.378  92.286 -22.369  1.00 36.47      C
ATOM   3637  O   CYS C  32      69.611  91.146 -22.819  1.00 33.53      C
ATOM   3638  CB  CYS C  32      70.840  93.110 -20.530  1.00 30.11      C
ATOM   3639  SG  CYS C  32      70.999  93.505 -18.757  1.00 30.29      C
ATOM   3640  N   SER C  33      68.922  93.383 -23.026  1.00 41.81      C
ATOM   3641  CA  SER C  33      69.024  93.272 -24.485  1.00 48.46      C
ATOM   3642  CB  SER C  33      68.136  94.544 -24.975  1.00 51.34      C
ATOM   3643  OG  SER C  33      68.752  95.734 -24.524  1.00 57.23      C
ATOM   3644  C   SER C  33      70.449  92.848 -24.842  1.00 54.01      C
ATOM   3645  O   SER C  33      71.347  92.852 -23.989  1.00 61.22      C
ATOM   3646  N   GLY C  34      70.633  92.487 -26.096  1.00 55.17      C
ATOM   3647  CA  GLY C  34      71.928  91.989 -26.558  1.00 49.56      C
ATOM   3648  C   GLY C  34      73.161  92.877 -26.748  1.00 47.38      C
ATOM   3649  O   GLY C  34      74.279  92.377 -26.942  1.00 46.07      C
ATOM   3650  N   THR C  35      72.832  94.184 -26.690  1.00 41.74      C
ATOM   3651  CA  THR C  35      73.932  95.134 -26.777  1.00 46.36      C
ATOM   3652  CB  THR C  35      73.603  96.329 -27.720  1.00 51.23      C
ATOM   3653  OG1 THR C  35      72.301  96.848 -27.419  1.00 57.47      C
ATOM   3654  CG2 THR C  35      73.641  95.881 -29.190  1.00 54.03      C
ATOM   3655  C   THR C  35      74.305  95.658 -25.383  1.00 48.56      C
ATOM   3656  O   THR C  35      75.001  96.655 -25.258  1.00 40.41      C
ATOM   3657  N   PHE C  36      73.840  94.969 -24.342  1.00 34.64      C
ATOM   3658  CA  PHE C  36      74.133  95.342 -22.965  1.00 31.17      C
ATOM   3659  CB  PHE C  36      72.888  95.857 -22.253  1.00 30.28      C
ATOM   3660  CG  PHE C  36      72.414  97.176 -22.750  1.00 32.70      C
ATOM   3661  CD1 PHE C  36      71.692  97.266 -23.944  1.00 36.40      C
ATOM   3662  CD2 PHE C  36      72.729  98.343 -22.054  1.00 33.13      C
ATOM   3663  CE1 PHE C  36      71.301  98.500 -24.427  1.00 37.59      C
ATOM   3664  CE2 PHE C  36      72.345  99.588 -22.528  1.00 32.44      C
ATOM   3665  CZ  PHE C  36      71.629  99.673 -23.718  1.00 38.52      C
ATOM   3666  C   PHE C  36      74.612  94.107 -22.239  1.00 34.05      C
ATOM   3667  O   PHE C  36      74.432  93.001 -22.727  1.00 31.93      C
ATOM   3668  N   ARG C  37      75.236  94.292 -21.079  1.00 28.78      C
ATOM   3669  CA  ARG C  37      75.703  93.167 -20.295  1.00 27.36      C
ATOM   3670  CB  ARG C  37      77.233  93.140 -20.235  1.00 27.49      C
ATOM   3671  CG  ARG C  37      77.871  92.816 -21.587  1.00 31.08      C
ATOM   3672  CD  ARG C  37      77.403  91.440 -22.049  1.00 27.97      C
ATOM   3673  NE  ARG C  37      78.050  91.042 -23.301  1.00 35.17      C
ATOM   3674  CZ  ARG C  37      77.641  91.427 -24.503  1.00 36.96      C
ATOM   3675  NH1 ARG C  37      76.572  92.213 -24.620  1.00 42.52      C
ATOM   3676  NH2 ARG C  37      78.308  91.039 -25.581  1.00 37.15      C
ATOM   3677  C   ARG C  37      75.091  93.309 -18.913  1.00 29.60      C
ATOM   3678  O   ARG C  37      75.060  94.400 -18.336  1.00 25.97      C
ATOM   3679  N   LEU C  38      74.614  92.193 -18.383  1.00 25.39      C
ATOM   3680  CA  LEU C  38      73.952  92.202 -17.083  1.00 27.27      C
ATOM   3681  CB  LEU C  38      73.038  90.984 -16.980  1.00 27.65      C
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ATOM	3682	CG	LEU	C	38	72.221	90.971	-15.692	1.00	35.28	C
ATOM	3683	CD1	LEU	C	38	70.799	91.354	-16.019	1.00	33.06	C
ATOM	3684	CD2	LEU	C	38	72.278	89.589	-15.051	1.00	40.58	C
ATOM	3685	C	LEU	C	38	74.951	92.203	-15.926	1.00	24.03	C
ATOM	3686	O	LEU	C	38	75.851	91.376	-15.892	1.00	27.79	C
ATOM	3687	N	ILE	C	39	74.794	93.146	-15.001	1.00	25.30	C
ATOM	3688	CA	ILE	C	39	75.654	93.264	-13.819	1.00	26.06	C
ATOM	3689	CB	ILE	C	39	76.255	94.707	-13.686	1.00	31.19	C
ATOM	3690	CG2	ILE	C	39	77.130	94.813	-12.455	1.00	28.28	C
ATOM	3691	CG1	ILE	C	39	77.057	95.071	-14.955	1.00	37.49	C
ATOM	3692	CD1	ILE	C	39	78.059	94.022	-15.415	1.00	46.78	C
ATOM	3693	C	ILE	C	39	74.787	92.979	-12.590	1.00	27.54	C
ATOM	3694	O	ILE	C	39	73.807	93.683	-12.327	1.00	21.11	C
ATOM	3695	N	GLY	C	40	75.140	91.950	-11.829	1.00	28.46	C
ATOM	3696	CA	GLY	C	40	74.351	91.619	-10.654	1.00	28.45	C
ATOM	3697	C	GLY	C	40	73.691	90.275	-10.901	1.00	31.11	C
ATOM	3698	O	GLY	C	40	73.762	89.752	-12.008	1.00	27.47	C
ATOM	3699	N	GLU	C	41	73.057	89.713	-9.876	1.00	32.89	C
ATOM	3700	CA	GLU	C	41	72.395	88.411	-9.994	1.00	37.70	C
ATOM	3701	CB	GLU	C	41	72.006	87.900	-8.597	1.00	35.85	C
ATOM	3702	CG	GLU	C	41	71.217	86.601	-8.624	1.00	47.53	C
ATOM	3703	CD	GLU	C	41	71.983	85.447	-9.235	1.00	48.84	C
ATOM	3704	OE1	GLU	C	41	71.419	84.733	-10.088	1.00	44.21	C
ATOM	3705	OE2	GLU	C	41	73.153	85.252	-8.842	1.00	56.75	C
ATOM	3706	C	GLU	C	41	71.161	88.510	-10.893	1.00	32.10	C
ATOM	3707	O	GLU	C	41	70.336	89.404	-10.718	1.00	31.37	C
ATOM	3708	N	LYS	C	42	71.033	87.604	-11.857	1.00	33.31	C
ATOM	3709	CA	LYS	C	42	69.879	87.647	-12.760	1.00	33.67	C
ATOM	3710	CB	LYS	C	42	70.207	86.955	-14.069	1.00	33.01	C
ATOM	3711	CG	LYS	C	42	70.550	85.515	-13.891	1.00	39.88	C
ATOM	3712	CD	LYS	C	42	70.862	84.895	-15.238	1.00	43.23	C
ATOM	3713	CE	LYS	C	42	71.922	83.820	-15.105	1.00	48.14	C
ATOM	3714	NZ	LYS	C	42	71.648	82.872	-13.965	1.00	52.44	C
ATOM	3715	C	LYS	C	42	68.591	87.038	-12.185	1.00	34.36	C
ATOM	3716	O	LYS	C	42	67.509	87.306	-12.687	1.00	37.69	C
ATOM	3717	N	SER	C	43	68.685	86.265	-11.117	1.00	25.52	C
ATOM	3718	CA	SER	C	43	67.472	85.664	-10.565	1.00	31.67	C
ATOM	3719	CB	SER	C	43	67.668	84.155	-10.331	1.00	28.31	C
ATOM	3720	OG	SER	C	43	67.869	83.464	-11.537	1.00	39.90	C
ATOM	3721	C	SER	C	43	67.099	86.274	-9.233	1.00	29.32	C
ATOM	3722	O	SER	C	43	67.945	86.318	-8.342	1.00	31.30	C
ATOM	3723	N	LEU	C	44	65.853	86.735	-9.087	1.00	27.40	C
ATOM	3724	CA	LEU	C	44	65.393	87.267	-7.808	1.00	28.37	C
ATOM	3725	CB	LEU	C	44	64.744	88.638	-7.931	1.00	27.60	C
ATOM	3726	CG	LEU	C	44	65.498	89.876	-8.393	1.00	38.75	C
ATOM	3727	CD1	LEU	C	44	64.700	91.149	-7.896	1.00	26.06	C
ATOM	3728	CD2	LEU	C	44	66.913	89.846	-7.907	1.00	39.16	C
ATOM	3729	C	LEU	C	44	64.352	86.315	-7.218	1.00	29.49	C
ATOM	3730	O	LEU	C	44	63.469	85.796	-7.914	1.00	35.15	C
ATOM	3731	N	LEU	C	45	64.434	86.137	-5.919	1.00	25.55	C
ATOM	3732	CA	LEU	C	45	63.560	85.222	-5.230	1.00	28.43	C
ATOM	3733	CB	LEU	C	45	64.412	84.210	-4.469	1.00	28.67	C
ATOM	3734	CG	LEU	C	45	63.709	83.269	-3.493	1.00	30.62	C
ATOM	3735	CD1	LEU	C	45	62.896	82.195	-4.244	1.00	32.56	C
ATOM	3736	CD2	LEU	C	45	64.798	82.623	-2.649	1.00	31.55	C

ATOM	3737	C	LEU	C	45	62.664	85.961	-4.263	1.00	28.71	C
ATOM	3738	O	LEU	C	45	63.094	86.894	-3.558	1.00	21.68	C
ATOM	3739	N	CYS	C	46	61.410	85.547	-4.238	1.00	25.91	C
ATOM	3740	CA	CYS	C	46	60.455	86.152	-3.343	1.00	26.90	C
ATOM	3741	C	CYS	C	46	60.610	85.392	-2.032	1.00	30.25	C
ATOM	3742	O	CYS	C	46	60.448	84.173	-1.980	1.00	28.51	C
ATOM	3743	CB	CYS	C	46	59.021	86.026	-3.908	1.00	28.02	C
ATOM	3744	SG	CYS	C	46	57.741	86.546	-2.696	1.00	28.63	C
ATOM	3745	N	ILE	C	47	60.925	86.115	-0.971	1.00	21.11	C
ATOM	3746	CA	ILE	C	47	61.120	85.484	0.314	1.00	24.65	C
ATOM	3747	CB	ILE	C	47	62.619	85.501	0.722	1.00	32.62	C
ATOM	3748	CG2	ILE	C	47	63.505	84.878	-0.358	1.00	27.06	C
ATOM	3749	CG1	ILE	C	47	63.050	86.958	0.959	1.00	25.64	C
ATOM	3750	CD1	ILE	C	47	64.429	87.119	1.592	1.00	32.03	C
ATOM	3751	C	ILE	C	47	60.431	86.274	1.421	1.00	31.05	C
ATOM	3752	O	ILE	C	47	59.931	87.399	1.226	1.00	22.58	C
ATOM	3753	N	THR	C	48	60.421	85.669	2.596	1.00	27.58	C
ATOM	3754	CA	THR	C	48	59.964	86.388	3.764	1.00	27.51	C
ATOM	3755	CB	THR	C	48	58.584	85.987	4.273	1.00	28.85	C
ATOM	3756	OG1	THR	C	48	58.303	86.778	5.426	1.00	25.48	C
ATOM	3757	CG2	THR	C	48	58.490	84.526	4.619	1.00	26.50	C
ATOM	3758	C	THR	C	48	61.001	86.164	4.839	1.00	29.22	C
ATOM	3759	O	THR	C	48	61.455	85.049	5.060	1.00	29.40	C
ATOM	3760	N	LYS	C	49	61.445	87.243	5.463	1.00	27.29	C
ATOM	3761	CA	LYS	C	49	62.425	87.112	6.522	1.00	31.22	C
ATOM	3762	CB	LYS	C	49	63.478	88.220	6.427	1.00	26.53	C
ATOM	3763	CG	LYS	C	49	64.229	88.239	5.134	1.00	35.41	C
ATOM	3764	CD	LYS	C	49	65.703	88.351	5.346	1.00	40.12	C
ATOM	3765	CE	LYS	C	49	66.262	87.134	6.055	1.00	42.30	C
ATOM	3766	NZ	LYS	C	49	67.729	87.262	6.166	1.00	46.64	C
ATOM	3767	C	LYS	C	49	61.745	87.219	7.877	1.00	33.53	C
ATOM	3768	O	LYS	C	49	62.249	86.692	8.856	1.00	30.36	C
ATOM	3769	N	ASP	C	50	60.596	87.896	7.952	1.00	25.34	C
ATOM	3770	CA	ASP	C	50	59.978	88.083	9.253	1.00	26.98	C
ATOM	3771	CB	ASP	C	50	59.961	89.579	9.597	1.00	25.16	C
ATOM	3772	CG	ASP	C	50	59.154	90.397	8.607	1.00	27.41	C
ATOM	3773	OD1	ASP	C	50	58.459	89.768	7.749	1.00	22.49	C
ATOM	3774	OD2	ASP	C	50	59.207	91.664	8.693	1.00	26.37	C
ATOM	3775	C	ASP	C	50	58.598	87.492	9.365	1.00	25.28	C
ATOM	3776	O	ASP	C	50	57.883	87.770	10.321	1.00	24.69	C
ATOM	3777	N	LYS	C	51	58.247	86.664	8.386	1.00	26.19	C
ATOM	3778	CA	LYS	C	51	56.948	86.006	8.319	1.00	23.97	C
ATOM	3779	CB	LYS	C	51	56.717	85.091	9.526	1.00	31.09	C
ATOM	3780	CG	LYS	C	51	57.749	84.021	9.749	1.00	32.84	C
ATOM	3781	CD	LYS	C	51	57.625	82.919	8.769	1.00	44.47	C
ATOM	3782	CE	LYS	C	51	58.505	81.752	9.179	1.00	52.55	C
ATOM	3783	NZ	LYS	C	51	58.266	81.397	10.605	1.00	51.40	C
ATOM	3784	C	LYS	C	51	55.791	86.996	8.241	1.00	25.78	C
ATOM	3785	O	LYS	C	51	54.660	86.628	8.510	1.00	25.03	C
ATOM	3786	N	VAL	C	52	56.048	88.252	7.896	1.00	25.78	C
ATOM	3787	CA	VAL	C	52	54.937	89.195	7.758	1.00	23.31	C
ATOM	3788	CB	VAL	C	52	54.976	90.286	8.894	1.00	30.82	C
ATOM	3789	CG1	VAL	C	52	53.786	91.197	8.802	1.00	27.39	C
ATOM	3790	CG2	VAL	C	52	54.946	89.611	10.264	1.00	33.79	C
ATOM	3791	C	VAL	C	52	55.085	89.832	6.376	1.00	29.16	C

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ATOM   3792  O   VAL C  52      54.193  89.764   5.537  1.00 25.28      C
ATOM   3793  N   ASP C  53      56.248  90.433   6.146  1.00 31.64      C
ATOM   3794  CA  ASP C  53      56.575  91.099   4.892  1.00 27.94      C
ATOM   3795  CB  ASP C  53      57.647  92.167   5.150  1.00 28.37      C
ATOM   3796  CG  ASP C  53      57.189  93.235   6.132  1.00 30.66      C
ATOM   3797  OD1 ASP C  53      56.323  94.069   5.744  1.00 20.78      C
ATOM   3798  OD2 ASP C  53      57.700  93.245   7.287  1.00 27.56      C
ATOM   3799  C   ASP C  53      57.112  90.126   3.837  1.00 23.86      C
ATOM   3800  O   ASP C  53      57.862  89.212   4.164  1.00 24.61      C
ATOM   3801  N   GLY C  54      56.735  90.327   2.573  1.00 26.63      C
ATOM   3802  CA  GLY C  54      57.253  89.489   1.476  1.00 20.87      C
ATOM   3803  C   GLY C  54      58.190  90.420   0.730  1.00 25.47      C
ATOM   3804  O   GLY C  54      57.814  91.563   0.435  1.00 19.97      C
ATOM   3805  N   THR C  55      59.422  89.999   0.459  1.00 22.42      C
ATOM   3806  CA  THR C  55      60.345  90.907  -0.247  1.00 21.92      C
ATOM   3807  CB  THR C  55      61.326  91.591   0.760  1.00 24.17      C
ATOM   3808  OG1 THR C  55      61.999  90.669   0.106  1.00 24.68      C
ATOM   3809  CG2 THR C  55      62.491  90.597   1.251  1.00 24.06      C
ATOM   3810  C   THR C  55      61.184  90.153  -1.284  1.00 22.33      C
ATOM   3811  O   THR C  55      61.298  88.929  -1.209  1.00 24.76      C
ATOM   3812  N   TRP C  56      61.767  90.882  -2.230  1.00 22.04      C
ATOM   3813  CA  TRP C  56      62.637  90.281  -3.226  1.00 21.23      C
ATOM   3814  CB  TRP C  56      62.689  91.142  -4.506  1.00 28.51      C
ATOM   3815  CG  TRP C  56      61.377  91.081  -5.223  1.00 25.63      C
ATOM   3816  CD2 TRP C  56      60.853  89.962  -5.970  1.00 26.11      C
ATOM   3817  CE2 TRP C  56      59.512  90.266  -6.287  1.00 23.40      C
ATOM   3818  CE3 TRP C  56      61.384  88.723  -6.383  1.00 25.94      C
ATOM   3819  CD1 TRP C  56      60.374  91.988  -5.141  1.00 23.59      C
ATOM   3820  NE1 TRP C  56      59.249  91.513  -5.771  1.00 25.69      C
ATOM   3821  CZ2 TRP C  56      58.679  89.384  -7.003  1.00 24.25      C
ATOM   3822  CZ3 TRP C  56      60.555  87.832  -7.095  1.00 26.08      C
ATOM   3823  CH2 TRP C  56      59.209  88.177  -7.398  1.00 29.68      C
ATOM   3824  C   TRP C  56      63.994  90.185  -2.504  1.00 22.58      C
ATOM   3825  O   TRP C  56      64.379  91.119  -1.805  1.00 23.17      C
ATOM   3826  N   ASP C  57      64.698  89.064  -2.660  1.00 24.44      C
ATOM   3827  CA  ASP C  57      65.949  88.838  -1.931  1.00 26.43      C
ATOM   3828  CB  ASP C  57      66.293  87.334  -1.894  1.00 26.66      C
ATOM   3829  CG  ASP C  57      65.722  86.762  -3.256  1.00 31.79      C
ATOM   3830  OD1 ASP C  57      67.166  85.599  -3.268  1.00 36.19      C
ATOM   3831  OD2 ASP C  57      66.613  87.435  -4.298  1.00 30.66      C
ATOM   3832  C   ASP C  57      67.173  89.647  -2.317  1.00 29.20      C
ATOM   3833  O   ASP C  57      68.161  89.651  -1.589  1.00 32.18      C
ATOM   3834  N   LYS C  58      67.084  90.363  -3.428  1.00 31.78      C
ATOM   3835  CA  LYS C  58      68.180  91.180  -3.928  1.00 31.51      C
ATOM   3836  CB  LYS C  58      69.091  90.366  -4.866  1.00 37.98      C
ATOM   3837  CG  LYS C  58      70.061  89.452  -4.166  1.00 49.29      C
ATOM   3838  CD  LYS C  58      69.648  87.987  -4.237  1.00 58.25      C
ATOM   3839  CE  LYS C  58      69.569  87.484  -5.686  1.00 55.39      C
ATOM   3840  NZ  LYS C  58      68.893  86.136  -5.803  1.00 46.73      C
ATOM   3841  C   LYS C  58      67.614  92.311  -4.741  1.00 29.28      C
ATOM   3842  O   LYS C  58      66.442  92.301  -5.106  1.00 29.16      C
ATOM   3843  N   PRO C  59      68.429  93.340  -4.958  1.00 32.29      C
ATOM   3844  CD  PRO C  59      69.835  93.582  -4.659  1.00 26.68      C
ATOM   3845  CA  PRO C  59      67.912  94.387  -5.841  1.00 24.28      C
ATOM   3846  CB  PRO C  59      68.919  95.530  -5.673  1.00 28.93      C
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ATOM   3847  CG  PRO C  59      70.198  94.856  -5.368  1.00 30.90      C
ATOM   3848  C   PRO C  59      67.949  93.982  -7.321  1.00 29.24      C
ATOM   3849  O   PRO C  59      68.694  93.012  -7.627  1.00 23.42      C
ATOM   3850  N   ALA C  60      67.208  94.594  -8.172  1.00 28.57      C
ATOM   3851  CA  ALA C  60      67.247  94.196  -9.570  1.00 31.26      C
ATOM   3852  CB  ALA C  60      66.284  95.039 -10.363  1.00 24.31      C
ATOM   3853  C   ALA C  60      68.674  94.376 -10.126  1.00 32.02      C
ATOM   3854  O   ALA C  60      69.403  95.259  -9.700  1.00 29.35      C
ATOM   3855  N   PRO C  61      69.101  93.498 -11.046  1.00 29.11      C
ATOM   3856  CD  PRO C  61      68.453  92.245 -11.466  1.00 26.65      C
ATOM   3857  CA  PRO C  61      70.449  93.643 -11.625  1.00 26.17      C
ATOM   3858  CB  PRO C  61      70.690  92.296 -12.307  1.00 28.95      C
ATOM   3859  CG  PRO C  61      69.280  91.838 -12.676  1.00 27.22      C
ATOM   3860  C   PRO C  61      70.327  94.810 -12.632  1.00 26.90      C
ATOM   3861  O   PRO C  61      69.221  95.303 -12.859  1.00 22.51      C
ATOM   3862  N   LYS C  62      71.430  95.290 -13.208  1.00 21.80      C
ATOM   3863  CA  LYS C  62      71.379  96.409 -14.158  1.00 24.26      C
ATOM   3864  CB  LYS C  62      72.173  97.615 -13.637  1.00 26.24      C
ATOM   3865  CG  LYS C  62      71.776  98.107 -12.246  1.00 39.00      C
ATOM   3866  CD  LYS C  62      71.465  99.585 -12.222  1.00 41.85      C
ATOM   3867  CE  LYS C  62      71.357 100.084 -10.800  1.00 46.78      C
ATOM   3868  NZ  LYS C  62      72.692 100.117 -10.118  1.00 55.22      C
ATOM   3869  C   LYS C  62      71.955  96.043 -15.507  1.00 21.61      C
ATOM   3870  O   LYS C  62      72.735  95.097 -15.607  1.00 25.68      C
ATOM   3871  N   CYS C  63      71.585  96.780 -16.549  1.00 27.02      C
ATOM   3872  CA  CYS C  63      72.113  96.526 -17.903  1.00 27.02      C
ATOM   3873  C   CYS C  63      73.118  97.601 -18.302  1.00 30.37      C
ATOM   3874  O   CYS C  63      72.751  98.756 -18.416  1.00 32.00      C
ATOM   3875  CB  CYS C  63      70.989  96.504 -18.932  1.00 28.91      C
ATOM   3876  SG  CYS C  63      69.851  95.146 -18.602  1.00 29.20      C
ATOM   3877  N   GLU C  64      74.376  97.213 -18.514  1.00 23.24      C
ATOM   3878  CA  GLU C  64      75.417  98.167 -18.890  1.00 30.86      C
ATOM   3879  CB  GLU C  64      76.707  97.873 -18.098  1.00 31.31      C
ATOM   3880  CG  GLU C  64      77.231  99.023 -17.228  1.00 39.58      C
ATOM   3881  CD  GLU C  64      78.383  98.616 -16.287  1.00 40.40      C
ATOM   3882  OE1 GLU C  64      79.134  97.679 -16.620  1.00 26.79      C
ATOM   3883  OE2 GLU C  64      78.543  99.233 -15.208  1.00 48.25      C
ATOM   3884  C   GLU C  64      75.703  98.022 -20.380  1.00 25.87      C
ATOM   3885  O   GLU C  64      75.849  96.903 -20.882  1.00 19.45      C
ATOM   3886  N   TYR C  65      75.782  99.155 -21.093  1.00 25.32      C
ATOM   3887  CA  TYR C  65      76.106  99.110 -22.530  1.00 31.90      C
ATOM   3888  CB  TYR C  65      76.325 100.536 -23.061  1.00 36.00      C
ATOM   3889  CG  TYR C  65      76.254 100.650 -24.570  1.00 42.53      C
ATOM   3890  CD1 TYR C  65      75.041 100.470 -25.238  1.00 42.78      C
ATOM   3891  CE1 TYR C  65      74.951 100.568 -26.621  1.00 40.68      C
ATOM   3892  CD2 TYR C  65      77.396 100.937 -25.331  1.00 48.40      C
ATOM   3893  CE2 TYR C  65      77.321 101.040 -26.729  1.00 48.66      C
ATOM   3894  CZ  TYR C  65      76.086 100.848 -27.366  1.00 48.38      C
ATOM   3895  OH  TYR C  65      75.998 100.947 -28.750  1.00 49.96      C
ATOM   3896  C   TYR C  65      77.407  98.304 -22.704  1.00 26.60      C
ATOM   3897  O   TYR C  65      78.410  98.624 -22.101  1.00 27.68      C
ATOM   3898  N   PHE C  66      77.404  97.279 -23.541  1.00 24.63      C
ATOM   3899  CA  PHE C  66      78.583  96.428 -23.736  1.00 25.64      C
ATOM   3900  CB  PHE C  66      78.250  95.339 -24.776  1.00 30.86      C
ATOM   3901  CG  PHE C  66      79.408  94.427 -25.130  1.00 30.23      C
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	ATOM	3902	CD1	PHE	C	66	80.137	93.775	-24.143	1.00	25.24	C
	ATOM	3903	CD2	PHE	C	66	79.753	94.208	-26.481	1.00	33.99	C
	ATOM	3904	CE1	PHE	C	66	81.206	92.899	-24.478	1.00	28.31	C
	ATOM	3905	CE2	PHE	C	66	80.822	93.329	-26.838	1.00	29.10	C
5	ATOM	3906	CZ	PHE	C	66	81.550	92.672	-25.826	1.00	27.94	C
	ATOM	3907	C	PHE	C	66	79.896	97.121	-24.133	1.00	32.19	C
	ATOM	3908	O	PHE	C	66	79.931	97.955	-25.044	1.00	29.06	C
	ATOM	3909	N	ASN	C	67	80.977	96.766	-23.440	1.00	25.19	C
	ATOM	3910	CA	ASN	C	67	82.297	97.296	-23.754	1.00	27.44	C
10	ATOM	3911	CB	ASN	C	67	82.845	98.203	-22.639	1.00	28.12	C
	ATOM	3912	CG	ASN	C	67	84.126	98.921	-23.066	1.00	33.33	C
	ATOM	3913	OD1	ASN	C	67	84.904	98.390	-23.870	1.00	27.62	C
	ATOM	3914	ND2	ASN	C	67	84.356	100.126	-22.528	1.00	28.36	C
	ATOM	3915	C	ASN	C	67	83.245	96.106	-23.942	1.00	30.05	C
15	ATOM	3916	O	ASN	C	67	83.706	95.489	-22.967	1.00	18.34	C
	ATOM	3917	N	LYS	C	68	83.565	95.816	-25.199	1.00	24.67	C
	ATOM	3918	CA	LYS	C	68	84.428	94.686	-25.511	1.00	29.80	C
	ATOM	3919	CB	LYS	C	68	84.491	94.441	-27.024	1.00	29.48	C
	ATOM	3920	CG	LYS	C	68	85.095	95.574	-27.875	1.00	39.59	C
20	ATOM	3921	CD	LYS	C	68	85.233	95.076	-29.326	1.00	45.75	C
	ATOM	3922	CE	LYS	C	68	85.993	96.016	-30.254	1.00	52.45	C
	ATOM	3923	NZ	LYS	C	68	85.111	96.916	-31.073	1.00	56.09	C
	ATOM	3924	C	LYS	C	68	85.821	94.831	-24.995	1.00	32.29	C
	ATOM	3925	O	LYS	C	68	86.541	93.833	-24.921	1.00	27.75	C
25	ATOM	3926	N	TYR	C	69	86.237	96.059	-24.663	1.00	25.84	C
	ATOM	3927	CA	TYR	C	69	87.599	96.229	-24.153	1.00	24.63	C
	ATOM	3928	CB	TYR	C	69	88.147	97.625	-24.434	1.00	27.26	C
	ATOM	3929	CG	TYR	C	69	88.161	97.948	-25.876	1.00	31.88	C
	ATOM	3930	CD1	TYR	C	69	87.105	98.635	-26.441	1.00	25.30	C
30	ATOM	3931	CE1	TYR	C	69	87.067	98.885	-27.791	1.00	33.19	C
	ATOM	3932	CD2	TYR	C	69	89.213	97.503	-26.708	1.00	32.15	C
	ATOM	3933	CE2	TYR	C	69	89.186	97.749	-28.079	1.00	32.52	C
	ATOM	3934	CZ	TYR	C	69	88.095	98.453	-28.614	1.00	34.98	C
	ATOM	3935	OH	TYR	C	69	88.031	98.764	-29.952	1.00	32.72	C
35	ATOM	3936	C	TYR	C	69	87.687	95.997	-22.673	1.00	30.29	C
	ATOM	3937	O	TYR	C	69	88.777	95.781	-22.158	1.00	28.03	C
	ATOM	3938	N	SER	C	70	86.565	96.050	-21.967	1.00	29.29	C
	ATOM	3939	CA	SER	C	70	86.597	95.868	-20.505	1.00	23.26	C
	ATOM	3940	CB	SER	C	70	85.204	96.061	-19.871	1.00	25.19	C
40	ATOM	3941	OG	SER	C	70	84.518	97.144	-20.277	1.00	30.67	C
	ATOM	3942	C	SER	C	70	87.175	94.504	-20.128	1.00	29.31	C
	ATOM	3943	O	SER	C	70	86.714	93.455	-20.641	1.00	33.25	C
	ATOM	3944	N	SER	C	71	88.113	94.596	-19.092	1.00	34.01	C
	ATOM	3945	CA	SER	C	71	88.825	93.422	-18.570	1.00	33.07	C
45	ATOM	3946	CB	SER	C	71	90.139	93.197	-19.314	1.00	37.09	C
	ATOM	3947	OG	SER	C	71	90.774	91.992	-18.919	1.00	36.97	C
	ATOM	3948	C	SER	C	71	89.145	93.621	-17.099	1.00	31.37	C
	ATOM	3949	O	SER	C	71	89.965	94.464	-16.748	1.00	31.95	C
	ATOM	3950	N	CYS	C	72	88.518	92.836	-16.230	1.00	32.50	C
50	ATOM	3951	CA	CYS	C	72	88.760	92.984	-14.803	1.00	31.24	C
	ATOM	3952	C	CYS	C	72	89.899	92.131	-14.294	1.00	32.97	C
	ATOM	3953	O	CYS	C	72	90.062	90.989	-14.695	1.00	37.51	C
	ATOM	3954	CB	CYS	C	72	87.479	92.670	-14.032	1.00	31.14	C
	ATOM	3955	SG	CYS	C	72	86.104	93.792	-14.488	1.00	35.33	C
55	ATOM	3956	N	PRO	C	73	90.723	92.681	-13.401	1.00	31.28	C

ATOM	3957	CD	PRO	C	73	90.688	94.015	-12.785	1.00	34.25	C
ATOM	3958	CA	PRO	C	73	91.836	91.900	-12.875	1.00	37.83	C
ATOM	3959	CB	PRO	C	73	92.700	92.953	-12.199	1.00	39.00	C
ATOM	3960	CG	PRO	C	73	91.667	93.862	-11.635	1.00	36.58	C
ATOM	3961	C	PRO	C	73	91.325	90.889	-11.872	1.00	40.84	C
ATOM	3962	O	PRO	C	73	90.265	91.088	-11.284	1.00	40.57	C
ATOM	3963	N	GLU	C	74	92.185	89.834	-11.599	1.00	44.75	C
ATOM	3964	CA	GLU	C	74	91.750	88.788	-10.731	1.00	50.06	C
ATOM	3965	CB	GLU	C	74	92.854	87.743	-10.680	1.00	55.68	C
ATOM	3966	CG	GLU	C	74	93.109	86.845	-9.771	1.00	64.35	C
ATOM	3967	CD	GLU	C	74	92.171	85.710	-10.135	1.00	67.16	C
ATOM	3968	OE1	GLU	C	74	92.147	85.315	-11.320	1.00	67.98	C
ATOM	3969	OE2	GLU	C	74	91.459	85.216	-9.236	1.00	69.43	C
ATOM	3970	C	GLU	C	74	91.482	89.377	-9.347	1.00	45.69	C
ATOM	3971	O	GLU	C	74	92.282	90.168	-8.832	1.00	43.16	C
ATOM	3972	N	PRO	C	75	90.195	89.176	-8.898	1.00	45.27	C
ATOM	3973	CD	PRO	C	75	89.118	88.373	-9.504	1.00	46.99	C
ATOM	3974	CA	PRO	C	75	89.789	89.765	-7.622	1.00	46.84	C
ATOM	3975	CB	PRO	C	75	88.278	89.575	-7.643	1.00	45.59	C
ATOM	3976	CG	PRO	C	75	88.129	88.251	-8.380	1.00	43.10	C
ATOM	3977	C	PRO	C	75	90.484	88.987	-6.471	1.00	46.31	C
ATOM	3978	O	PRO	C	75	90.622	87.764	-6.533	1.00	43.58	C
ATOM	3979	N	ILE	C	76	90.967	89.682	-5.452	1.00	44.06	C
ATOM	3980	CA	ILE	C	76	91.585	88.961	-4.346	1.00	49.43	C
ATOM	3981	CB	ILE	C	76	93.091	89.252	-4.220	1.00	50.66	C
ATOM	3982	CG2	ILE	C	76	93.648	88.589	-2.960	1.00	51.02	C
ATOM	3983	CG1	ILE	C	76	93.829	88.692	-5.433	1.00	53.97	C
ATOM	3984	CD1	ILE	C	76	95.327	88.938	-5.393	1.00	58.58	C
ATOM	3985	C	ILE	C	76	90.910	89.320	-3.041	1.00	47.38	C
ATOM	3986	O	ILE	C	76	90.663	90.496	-2.770	1.00	45.77	C
ATOM	3987	N	VAL	C	77	90.596	88.303	-2.240	1.00	47.49	C
ATOM	3988	CA	VAL	C	77	89.933	88.516	-0.949	1.00	47.30	C
ATOM	3989	CB	VAL	C	77	88.466	87.930	-0.945	1.00	46.81	C
ATOM	3990	CG1	VAL	C	77	87.848	88.039	0.474	1.00	43.39	C
ATOM	3991	CG2	VAL	C	77	87.604	88.654	-1.986	1.00	42.04	C
ATOM	3992	C	VAL	C	77	90.725	87.855	0.188	1.00	47.58	C
ATOM	3993	O	VAL	C	77	90.823	86.620	0.263	1.00	45.09	C
ATOM	3994	N	PRO	C	78	91.301	88.669	1.086	1.00	44.97	C
ATOM	3995	CD	PRO	C	78	91.365	90.140	1.032	1.00	45.60	C
ATOM	3996	CA	PRO	C	78	92.078	88.143	2.221	1.00	44.08	C
ATOM	3997	CB	PRO	C	78	92.461	89.407	2.989	1.00	45.76	C
ATOM	3998	CG	PRO	C	78	92.593	90.447	1.892	1.00	46.76	C
ATOM	3999	C	PRO	C	78	91.208	87.217	3.065	1.00	43.84	C
ATOM	4000	O	PRO	C	78	90.088	87.568	3.403	1.00	43.30	C
ATOM	4001	N	GLY	C	79	91.705	86.035	3.395	1.00	44.80	C
ATOM	4002	CA	GLY	C	79	90.913	85.126	4.204	1.00	43.45	C
ATOM	4003	C	GLY	C	79	89.868	84.402	3.379	1.00	45.18	C
ATOM	4004	O	GLY	C	79	89.025	83.667	3.914	1.00	43.18	C
ATOM	4005	N	GLY	C	80	89.922	84.605	2.067	1.00	41.25	C
ATOM	4006	CA	GLY	C	80	88.970	83.946	1.185	1.00	39.64	C
ATOM	4007	C	GLY	C	80	89.622	83.287	-0.022	1.00	44.23	C
ATOM	4008	O	GLY	C	80	90.827	83.420	-0.269	1.00	40.56	C
ATOM	4009	N	TYR	C	81	88.829	82.545	-0.779	1.00	42.62	C
ATOM	4010	CA	TYR	C	81	89.343	81.905	-1.973	1.00	46.24	C
ATOM	4011	CB	TYR	C	81	89.908	80.496	-1.655	1.00	44.92	C

ATOM	4012	CG	TYR	C	81	88.934	79.522	-1.020	1.00	46.64	C
ATOM	4013	CD1	TYR	C	81	88.405	78.463	-1.754	1.00	48.03	C
ATOM	4014	CE1	TYR	C	81	87.438	77.618	-1.221	1.00	48.43	C
ATOM	4015	CD2	TYR	C	81	88.478	79.709	0.281	1.00	47.96	C
ATOM	4016	CE2	TYR	C	81	87.503	78.871	0.826	1.00	50.43	C
ATOM	4017	CZ	TYR	C	81	86.980	77.827	0.062	1.00	51.08	C
ATOM	4018	OH	TYR	C	81	85.948	77.038	0.550	1.00	54.25	C
ATOM	4019	C	TYR	C	81	88.233	81.854	-3.028	1.00	50.13	C
ATOM	4020	O	TYR	C	81	87.039	81.840	-2.711	1.00	46.05	C
ATOM	4021	N	LYS	C	82	88.643	81.853	-4.289	1.00	50.32	C
ATOM	4022	CA	LYS	C	82	87.697	81.828	-5.380	1.00	53.74	C
ATOM	4023	CB	LYS	C	82	88.393	82.238	-6.681	1.00	53.51	C
ATOM	4024	CG	LYS	C	82	87.466	82.280	-7.884	1.00	54.66	C
ATOM	4025	CD	LYS	C	82	88.182	82.779	-9.126	1.00	52.50	C
ATOM	4026	CE	LYS	C	82	89.254	81.803	-9.563	1.00	53.91	C
ATOM	4027	NZ	LYS	C	82	90.030	82.321	-10.718	1.00	52.48	C
ATOM	4028	C	LYS	C	82	87.089	80.447	-5.528	1.00	54.39	C
ATOM	4029	O	LYS	C	82	87.782	79.435	-5.429	1.00	54.15	C
ATOM	4030	N	ILE	C	83	85.783	80.412	-5.740	1.00	53.36	C
ATOM	4031	CA	ILE	C	83	85.083	79.157	-5.935	1.00	56.28	C
ATOM	4032	CB	ILE	C	83	83.815	79.085	-5.070	1.00	57.52	C
ATOM	4033	CG2	ILE	C	83	82.803	78.186	-5.698	1.00	58.38	C
ATOM	4034	CG1	ILE	C	83	84.162	78.510	-3.702	1.00	59.41	C
ATOM	4035	CD1	ILE	C	83	85.312	79.203	-3.034	1.00	64.54	C
ATOM	4036	C	ILE	C	83	84.698	79.018	-7.408	1.00	60.57	C
ATOM	4037	O	ILE	C	83	84.790	77.926	-7.969	1.00	61.13	C
ATOM	4038	N	ARG	C	84	84.274	80.125	-8.025	1.00	58.19	C
ATOM	4039	CA	ARG	C	84	83.859	80.134	-9.432	1.00	55.53	C
ATOM	4040	CB	ARG	C	84	82.340	80.259	-9.557	1.00	59.40	C
ATOM	4041	CG	ARG	C	84	81.555	79.123	-8.937	1.00	66.78	C
ATOM	4042	CD	ARG	C	84	80.080	79.471	-8.783	1.00	70.71	C
ATOM	4043	NE	ARG	C	84	79.338	78.353	-8.204	1.00	78.80	C
ATOM	4044	CZ	ARG	C	84	78.041	78.384	-7.902	1.00	82.83	C
ATOM	4045	NH1	ARG	C	84	77.331	79.487	-8.124	1.00	84.17	C
ATOM	4046	NH2	ARG	C	84	77.454	77.308	-7.378	1.00	84.81	C
ATOM	4047	C	ARG	C	84	84.475	81.305	-10.156	1.00	54.05	C
ATOM	4048	O	ARG	C	84	84.812	82.313	-9.543	1.00	52.78	C
ATOM	4049	N	GLY	C	85	84.612	81.164	-11.468	1.00	51.61	C
ATOM	4050	CA	GLY	C	85	85.166	82.234	-12.265	1.00	52.64	C
ATOM	4051	C	GLY	C	85	86.542	81.935	-12.801	1.00	52.39	C
ATOM	4052	O	GLY	C	85	87.400	81.412	-12.093	1.00	53.26	C
ATOM	4053	N	SER	C	86	86.768	82.264	-14.063	1.00	56.65	C
ATOM	4054	CA	SER	C	86	88.074	82.013	-14.636	1.00	60.26	C
ATOM	4055	CB	SER	C	86	88.078	80.685	-15.393	1.00	63.40	C
ATOM	4056	OG	SER	C	86	89.410	80.222	-15.570	1.00	73.69	C
ATOM	4057	C	SER	C	86	88.182	83.126	-15.567	1.00	56.75	C
ATOM	4058	O	SER	C	86	87.650	83.698	-16.257	1.00	55.15	C
ATOM	4059	N	THR	C	87	89.775	83.428	-15.565	1.00	58.49	C
ATOM	4060	CA	THR	C	87	90.343	84.457	-16.417	1.00	57.84	C
ATOM	4061	CB	THR	C	87	91.816	84.711	-16.006	1.00	62.33	C
ATOM	4062	OG1	THR	C	87	91.873	85.892	-15.197	1.00	69.91	C
ATOM	4063	CG2	THR	C	87	92.724	84.863	-17.215	1.00	64.96	C
ATOM	4064	C	THR	C	87	90.257	84.034	-17.886	1.00	55.75	C
ATOM	4065	O	THR	C	87	90.241	82.842	-18.198	1.00	56.65	C
ATOM	4066	N	PRO	C	88	90.134	85.007	-18.805	1.00	52.96	C

ATOM	4067	CD	PRO	C	88	90.192	84.766	-20.259	1.00	53.18	C
ATOM	4068	CA	PRO	C	88	90.969	86.442	-18.533	1.00	52.06	C
ATOM	4069	CB	PRO	C	88	90.533	87.060	-19.849	1.00	50.34	C
ATOM	4070	CG	PRO	C	88	89.909	86.162	-20.842	1.00	52.45	C
ATOM	4071	C	PRO	C	88	88.630	86.844	-18.183	1.00	47.83	C
ATOM	4072	O	PRO	C	88	87.666	86.219	-18.628	1.00	43.02	C
ATOM	4073	N	TYR	C	89	88.592	87.903	-17.398	1.00	40.94	C
ATOM	4074	CA	TYR	C	89	87.294	88.376	-16.977	1.00	40.87	C
ATOM	4075	CB	TYR	C	89	87.276	88.839	-15.516	1.00	41.58	C
ATOM	4076	CG	TYR	C	89	87.696	87.730	-14.570	1.00	47.21	C
ATOM	4077	CD1	TYR	C	89	88.836	87.759	-13.879	1.00	48.57	C
ATOM	4078	CE1	TYR	C	89	89.260	86.711	-13.043	1.00	52.12	C
ATOM	4079	CD2	TYR	C	89	86.835	86.625	-14.397	1.00	47.83	C
ATOM	4080	CE2	TYR	C	89	87.203	85.573	-13.567	1.00	52.56	C
ATOM	4081	CZ	TYR	C	89	88.409	85.618	-12.892	1.00	52.86	C
ATOM	4082	OH	TYR	C	89	88.734	84.568	-12.059	1.00	55.18	C
ATOM	4083	C	TYR	C	89	86.775	89.516	-17.874	1.00	37.75	C
ATOM	4084	O	TYR	C	89	87.368	90.582	-17.837	1.00	35.86	C
ATOM	4085	N	ARG	C	90	85.742	89.282	-18.677	1.00	36.76	C
ATOM	4086	CA	ARG	C	90	85.227	90.291	-19.591	1.00	31.74	C
ATOM	4087	CB	ARG	C	90	84.956	89.672	-20.957	1.00	39.30	C
ATOM	4088	CG	ARG	C	90	86.211	89.526	-21.808	1.00	51.87	C
ATOM	4089	CD	ARG	C	90	86.600	88.085	-21.981	1.00	60.63	C
ATOM	4090	NE	ARG	C	90	87.619	87.933	-23.048	1.00	68.24	C
ATOM	4091	CZ	ARG	C	90	88.091	86.767	-23.501	1.00	68.54	C
ATOM	4092	NH1	ARG	C	90	87.673	85.604	-22.993	1.00	64.59	C
ATOM	4093	NH2	ARG	C	90	88.987	86.767	-24.479	1.00	70.32	C
ATOM	4094	C	ARG	C	90	83.959	90.915	-19.048	1.00	31.15	C
ATOM	4095	O	ARG	C	90	83.414	90.456	-18.040	1.00	24.92	C
ATOM	4096	N	HIS	C	91	83.493	91.955	-19.725	1.00	23.82	C
ATOM	4097	CA	HIS	C	91	82.085	92.674	-19.301	1.00	23.05	C
ATOM	4098	CB	HIS	C	91	81.872	93.640	-20.406	1.00	26.29	C
ATOM	4099	CG	HIS	C	91	80.849	94.665	-19.998	1.00	23.49	C
ATOM	4100	CD2	HIS	C	91	80.142	95.553	-20.744	1.00	20.45	C
ATOM	4101	ND1	HIS	C	91	80.515	94.920	-18.685	1.00	28.99	C
ATOM	4102	CE1	HIS	C	91	79.651	95.923	-18.637	1.00	19.30	C
ATOM	4103	NE2	HIS	C	91	79.412	96.325	-19.873	1.00	28.70	C
ATOM	4104	C	HIS	C	91	81.142	91.717	-19.003	1.00	24.93	C
ATOM	4105	O	HIS	C	91	80.771	90.926	-19.862	1.00	22.92	C
ATOM	4106	N	GLY	C	92	80.575	91.808	-17.801	1.00	25.08	C
ATOM	4107	CA	GLY	C	92	79.459	90.949	-17.435	1.00	25.83	C
ATOM	4108	C	GLY	C	92	79.834	89.612	-16.803	1.00	26.66	C
ATOM	4109	O	GLY	C	92	78.964	88.947	-16.233	1.00	30.96	C
ATOM	4110	N	ASP	C	93	81.098	89.203	-16.913	1.00	24.69	C
ATOM	4111	CA	ASP	C	93	81.558	87.940	-16.311	1.00	28.03	C
ATOM	4112	CB	ASP	C	93	83.001	87.609	-16.749	1.00	26.26	C
ATOM	4113	CG	ASP	C	93	83.101	87.123	-18.214	1.00	33.28	C
ATOM	4114	OD1	ASP	C	93	84.243	86.973	-18.725	1.00	35.30	C
ATOM	4115	OD2	ASP	C	93	82.056	86.995	-18.859	1.00	33.91	C
ATOM	4116	C	ASP	C	93	81.535	88.080	-14.791	1.00	32.16	C
ATOM	4117	O	ASP	C	93	81.641	89.197	-14.254	1.00	32.11	C
ATOM	4118	N	SER	C	94	81.400	86.966	-14.082	1.00	27.90	C
ATOM	4119	CA	SER	C	94	81.395	87.050	-12.632	1.00	37.96	C
ATOM	4120	CB	SER	C	94	79.983	86.889	-12.104	1.00	35.76	C
ATOM	4121	OG	SER	C	94	79.577	85.556	-12.314	1.00	39.23	C

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ATOM   4122  C   SER C  94      82.287  85.986 -11.997  1.00 38.51      C
ATOM   4123  O   SER C  94      82.713  85.038 -12.655  1.00 36.22      C
ATOM   4124  N   VAL C  95      82.550  86.154 -10.706  1.00 38.03      C
ATOM   4125  CA  VAL C  95      83.373  85.221  -9.943  1.00 42.81      C
ATOM   4126  CB  VAL C  95      84.825  85.728  -9.743  1.00 41.37      C
ATOM   4127  CG1 VAL C  95      85.454  86.096 -11.073  1.00 46.63      C
ATOM   4128  CG2 VAL C  95      84.840  86.960  -8.916  1.00 36.92      C
ATOM   4129  C   VAL C  95      82.724  89.111  -8.587  1.00 43.66      C
ATOM   4130  O   VAL C  95      82.023  86.024  -8.155  1.00 43.47      C
ATOM   4131  N   THR C  96      82.939  83.988  -7.918  1.00 45.64      C
ATOM   4132  CA  THR C  96      82.356  83.806  -6.599  1.00 46.87      C
ATOM   4133  CB  THR C  96      81.258  82.736  -6.600  1.00 46.87      C
ATOM   4134  OG1 THR C  96      80.233  83.101  -7.531  1.00 40.12      C
ATOM   4135  CG2 THR C  96      80.635  82.635  -5.208  1.00 50.66      C
ATOM   4136  C   THR C  96      83.432  83.403  -5.612  1.00 43.20      C
ATOM   4137  O   THR C  96      84.363  82.686  -5.962  1.00 41.73      C
ATOM   4138  N   PHE C  97      83.302  83.886  -4.387  1.00 39.07      C
ATOM   4139  CA  PHE C  97      84.267  83.578  -3.349  1.00 43.95      C
ATOM   4140  CB  PHE C  97      84.898  84.854  -2.810  1.00 45.41      C
ATOM   4141  CG  PHE C  97      85.850  85.519  -3.750  1.00 46.14      C
ATOM   4142  CD1 PHE C  97      85.422  86.543  -4.594  1.00 42.85      C
ATOM   4143  CD2 PHE C  97      87.195  85.162  -3.749  1.00 45.67      C
ATOM   4144  CE1 PHE C  97      86.320  87.194  -5.406  1.00 39.79      C
ATOM   4145  CE2 PHE C  97      88.101  85.812  -4.562  1.00 42.72      C
ATOM   4146  CZ  PHE C  97      87.663  86.829  -5.390  1.00 41.65      C
ATOM   4147  C   PHE C  97      83.646  82.859  -2.158  1.00 46.38      C
ATOM   4148  O   PHE C  97      82.421  82.804  -1.988  1.00 39.27      C
ATOM   4149  N   ALA C  98      84.530  82.332  -1.318  1.00 48.32      C
ATOM   4150  CA  ALA C  98      84.155  81.664  -0.076  1.00 46.94      C
ATOM   4151  CB  ALA C  98      84.112  80.158  -0.277  1.00 46.22      C
ATOM   4152  C   ALA C  98      85.254  82.038   0.929  1.00 46.65      C
ATOM   4153  O   ALA C  98      86.394  82.293   0.536  1.00 44.10      C
ATOM   4154  N   CYS C  99      84.914  82.303   2.212  1.00 46.08      C
ATOM   4155  CA  CYS C  99      85.917  82.423   3.209  1.00 47.08      C
ATOM   4156  C   CYS C  99      85.590  81.156   3.711  1.00 46.05      C
ATOM   4157  O   CYS C  99      85.963  80.096   3.760  1.00 43.34      C
ATOM   4158  CB  CYS C  99      85.289  83.158   4.375  1.00 44.52      C
ATOM   4159  SG  CYS C  99      84.727  84.809   3.844  1.00 44.83      C
ATOM   4160  N   LYS C 100      87.874  81.273   4.056  1.00 47.36      C
ATOM   4161  CA  LYS C 100      88.645  80.147   4.574  1.00 48.81      C
ATOM   4162  CB  LYS C 100      90.135  80.489   4.594  1.00 49.39      C
ATOM   4163  CG  LYS C 100      90.750  80.658   3.219  1.00 54.21      C
ATOM   4164  CD  LYS C 100      92.190  81.114   3.317  1.00 54.87      C
ATOM   4165  CE  LYS C 100      92.806  81.267   1.942  1.00 57.13      C
ATOM   4166  NZ  LYS C 100      94.197  81.768   2.053  1.00 60.72      C
ATOM   4167  C   LYS C 100      88.165  79.861   5.997  1.00 49.95      C
ATOM   4168  O   LYS C 100      87.495  80.705   6.619  1.00 48.69      C
ATOM   4169  N   THR C 101      88.786  78.765   6.373  1.00 51.22      C
ATOM   4170  CA  THR C 101      88.580  78.224   7.709  1.00 55.29      C
ATOM   4171  CB  THR C 101      89.528  77.069   8.012  1.00 57.10      C
ATOM   4172  OG1 THR C 101      89.306  76.008   7.077  1.00 64.35      C
ATOM   4173  CG2 THR C 101      89.308  76.559   9.429  1.00 57.34      C
ATOM   4174  C   THR C 101      88.780  79.304   8.764  1.00 49.93      C
ATOM   4175  O   THR C 101      89.894  79.947   8.793  1.00 47.27      C
ATOM   4176  N   ASN C 102      88.004  79.652   9.763  1.00 46.86      C
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ATOM	4177	CA	ASN	C	102	88.149	80.670	10.780	1.00	48.18	C
ATOM	4178	CB	ASN	C	102	89.557	80.629	11.363	1.00	46.95	C
ATOM	4179	CG	ASN	C	102	89.845	79.289	12.014	1.00	48.40	C
ATOM	4180	OD1	ASN	C	102	88.985	78.720	12.693	1.00	41.35	C
ATOM	4181	ND2	ASN	C	102	91.051	78.775	11.810	1.00	49.40	C
ATOM	4182	C	ASN	C	102	87.761	82.030	10.236	1.00	49.20	C
ATOM	4183	O	ASN	C	102	88.252	83.052	10.922	1.00	46.49	C
ATOM	4184	N	PHE	C	103	87.220	82.295	9.176	1.00	48.20	C
ATOM	4185	CA	PHE	C	103	86.584	83.570	8.755	1.00	49.30	C
ATOM	4186	CB	PHE	C	103	87.390	84.074	7.554	1.00	46.94	C
ATOM	4187	CG	PHE	C	103	88.859	84.187	7.814	1.00	45.01	C
ATOM	4188	CD1	PHE	C	103	89.671	83.059	7.792	1.00	48.38	C
ATOM	4189	CD2	PHE	C	103	89.437	85.421	8.082	1.00	48.98	C
ATOM	4190	CE1	PHE	C	103	91.045	83.157	8.034	1.00	48.94	C
ATOM	4191	CE2	PHE	C	103	90.810	85.533	8.328	1.00	48.39	C
ATOM	4192	CZ	PHE	C	103	91.616	84.400	8.302	1.00	46.82	C
ATOM	4193	C	PHE	C	103	85.097	83.521	8.378	1.00	50.21	C
ATOM	4194	O	PHE	C	103	84.570	82.478	7.968	1.00	49.82	C
ATOM	4195	N	SER	C	104	84.414	84.647	8.565	1.00	48.66	C
ATOM	4196	CA	SER	C	104	83.012	84.745	8.214	1.00	45.33	C
ATOM	4197	CB	SER	C	104	82.165	85.191	9.417	1.00	46.37	C
ATOM	4198	OG	SER	C	104	82.048	86.605	9.522	1.00	57.43	C
ATOM	4199	C	SER	C	104	82.984	85.792	7.108	1.00	41.51	C
ATOM	4200	O	SER	C	104	83.757	86.736	7.130	1.00	38.53	C
ATOM	4201	N	MET	C	105	82.114	85.616	6.129	1.00	41.72	C
ATOM	4202	CA	MET	C	105	82.036	86.573	5.038	1.00	43.60	C
ATOM	4203	CB	MET	C	105	81.601	85.872	3.748	1.00	44.67	C
ATOM	4204	CG	MET	C	105	81.330	86.830	2.579	1.00	40.80	C
ATOM	4205	SD	MET	C	105	80.914	85.922	1.118	1.00	45.07	C
ATOM	4206	CE	MET	C	105	82.489	85.186	0.675	1.00	39.55	C
ATOM	4207	C	MET	C	105	81.077	87.722	5.308	1.00	46.26	C
ATOM	4208	O	MET	C	105	79.972	87.519	5.816	1.00	44.17	C
ATOM	4209	N	ASN	C	106	81.518	88.927	4.963	1.00	47.38	C
ATOM	4210	CA	ASN	C	106	80.707	90.137	5.078	1.00	49.51	C
ATOM	4211	CB	ASN	C	106	81.391	91.160	5.984	1.00	56.07	C
ATOM	4212	CG	ASN	C	106	80.769	92.539	5.879	1.00	63.53	C
ATOM	4213	OD1	ASN	C	106	80.925	93.233	4.867	1.00	66.72	C
ATOM	4214	ND2	ASN	C	106	80.048	92.943	6.921	1.00	68.89	C
ATOM	4215	C	ASN	C	106	80.572	90.688	3.645	1.00	49.28	C
ATOM	4216	O	ASN	C	106	81.566	91.073	3.015	1.00	46.49	C
ATOM	4217	N	GLY	C	107	79.344	90.700	3.130	1.00	50.96	C
ATOM	4218	CA	GLY	C	107	79.102	91.178	1.776	1.00	47.29	C
ATOM	4219	C	GLY	C	107	78.620	90.074	0.846	1.00	46.96	C
ATOM	4220	O	GLY	C	107	78.421	88.940	1.275	1.00	48.97	C
ATOM	4221	N	ASN	C	108	78.439	90.398	-0.434	1.00	50.83	C
ATOM	4222	CA	ASN	C	108	77.974	89.429	-1.426	1.00	49.00	C
ATOM	4223	CB	ASN	C	108	77.392	90.148	-2.635	1.00	56.26	C
ATOM	4224	CG	ASN	C	108	76.392	91.180	-2.247	1.00	61.63	C
ATOM	4225	OD1	ASN	C	108	76.703	92.371	-2.168	1.00	67.56	C
ATOM	4226	ND2	ASN	C	108	75.176	90.735	-1.977	1.00	62.48	C
ATOM	4227	C	ASN	C	108	79.125	88.561	-1.887	1.00	46.12	C
ATOM	4228	O	ASN	C	108	80.217	89.064	-2.155	1.00	42.01	C
ATOM	4229	N	LYS	C	109	78.858	87.266	-2.016	1.00	38.69	C
ATOM	4230	CA	LYS	C	109	79.874	86.310	-2.407	1.00	41.12	C
ATOM	4231	CB	LYS	C	109	79.444	84.897	-2.023	1.00	44.04	C

ATOM	4232	CG	LYS	C	109	78.255	84.360	-2.804	1.00	45.47	C
ATOM	4233	CD	LYS	C	109	77.585	83.222	-2.019	1.00	51.74	C
ATOM	4234	CE	LYS	C	109	76.584	82.453	-2.865	1.00	59.58	C
ATOM	4235	NZ	LYS	C	109	77.262	81.664	-3.956	1.00	64.18	C
ATOM	4236	C	LYS	C	109	80.199	86.324	-3.874	1.00	40.75	C
ATOM	4237	O	LYS	C	109	81.189	85.714	-4.307	1.00	41.19	C
ATOM	4238	N	SER	C	110	79.358	86.988	-4.655	1.00	38.36	C
ATOM	4239	CA	SER	C	110	79.578	87.024	-6.101	1.00	36.23	C
ATOM	4240	CB	SER	C	110	78.437	86.305	-6.834	1.00	39.46	C
ATOM	4241	OG	SER	C	110	78.481	84.918	-6.579	1.00	36.52	C
ATOM	4242	C	SER	C	110	79.635	88.421	-6.581	1.00	29.42	C
ATOM	4243	O	SER	C	110	78.876	89.247	-6.098	1.00	28.55	C
ATOM	4244	N	VAL	C	111	80.560	88.692	-7.499	1.00	30.69	C
ATOM	4245	CA	VAL	C	111	80.678	90.017	-8.105	1.00	29.50	C
ATOM	4246	CB	VAL	C	111	81.934	90.782	-7.652	1.00	33.90	C
ATOM	4247	CG1	VAL	C	111	81.666	91.463	-6.325	1.00	32.11	C
ATOM	4248	CG2	VAL	C	111	83.135	89.825	-7.579	1.00	26.88	C
ATOM	4249	C	VAL	C	111	80.718	89.916	-9.632	1.00	29.99	C
ATOM	4250	O	VAL	C	111	80.996	88.853	-10.194	1.00	27.74	C
ATOM	4251	N	TRP	C	112	80.448	91.034	-10.299	1.00	25.72	C
ATOM	4252	CA	TRP	C	112	80.437	91.062	-11.756	1.00	25.20	C
ATOM	4253	CB	TRP	C	112	79.020	91.411	-12.237	1.00	26.69	C
ATOM	4254	CG	TRP	C	112	78.107	90.226	-12.146	1.00	33.54	C
ATOM	4255	CD2	TRP	C	112	77.481	89.706	-10.957	1.00	30.54	C
ATOM	4256	CE2	TRP	C	112	76.820	88.505	-11.322	1.00	33.04	C
ATOM	4257	CE3	TRP	C	112	77.421	90.133	-9.622	1.00	31.04	C
ATOM	4258	CD1	TRP	C	112	77.799	89.338	-13.158	1.00	37.78	C
ATOM	4259	NE1	TRP	C	112	77.029	88.309	-12.665	1.00	35.55	C
ATOM	4260	CZ2	TRP	C	112	76.110	87.729	-10.397	1.00	27.67	C
ATOM	4261	CZ3	TRP	C	112	76.713	89.357	-8.696	1.00	30.43	C
ATOM	4262	CH2	TRP	C	112	76.067	88.168	-9.092	1.00	26.78	C
ATOM	4263	C	TRP	C	112	81.456	92.052	-12.307	1.00	27.61	C
ATOM	4264	O	TRP	C	112	81.719	93.091	-11.701	1.00	22.47	C
ATOM	4265	N	CYS	C	113	82.042	91.719	-13.455	1.00	26.10	C
ATOM	4266	CA	CYS	C	113	83.025	92.593	-14.083	1.00	25.33	C
ATOM	4267	C	CYS	C	113	82.313	93.725	-14.830	1.00	30.04	C
ATOM	4268	O	CYS	C	113	81.611	93.488	-15.824	1.00	28.98	C
ATOM	4269	CB	CYS	C	113	83.897	91.780	-15.029	1.00	26.94	C
ATOM	4270	SG	CYS	C	113	85.096	92.793	-15.958	1.00	29.69	C
ATOM	4271	N	GLN	C	114	82.478	94.951	-14.336	1.00	22.99	C
ATOM	4272	CA	GLN	C	114	81.842	96.127	-14.927	1.00	25.16	C
ATOM	4273	CB	GLN	C	114	81.597	97.177	-13.835	1.00	28.73	C
ATOM	4274	CG	GLN	C	114	80.857	96.602	-12.630	1.00	36.89	C
ATOM	4275	CD	GLN	C	114	80.727	97.569	-11.457	1.00	42.08	C
ATOM	4276	OE1	GLN	C	114	79.802	98.365	-11.382	1.00	49.79	C
ATOM	4277	NE2	GLN	C	114	81.665	97.493	-10.539	1.00	49.11	C
ATOM	4278	C	GLN	C	114	82.630	96.739	-16.092	1.00	31.28	C
ATOM	4279	O	GLN	C	114	83.827	96.444	-16.284	1.00	27.94	C
ATOM	4280	N	ALA	C	115	81.956	97.594	-16.865	1.00	25.85	C
ATOM	4281	CA	ALA	C	115	82.564	98.246	-18.031	1.00	28.40	C
ATOM	4282	CB	ALA	C	115	81.577	99.211	-18.667	1.00	20.65	C
ATOM	4283	C	ALA	C	115	83.844	98.990	-17.651	1.00	28.38	C
ATOM	4284	O	ALA	C	115	84.797	99.004	-18.432	1.00	23.27	C
ATOM	4285	N	ASN	C	116	83.873	99.587	-16.456	1.00	23.81	C
ATOM	4286	CA	ASN	C	116	85.060	100.327	-16.002	1.00	28.02	C

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ATOM   4287  CB  ASN C 116      84.663 101.425 -14.993  1.00 28.32      C
ATOM   4288  CG  ASN C 116      83.983 100.858 -13.746  1.00 27.71      C
ATOM   4289  OD1 ASN C 116      84.129  99.674 -13.436  1.00 24.66      C
ATOM   4290  ND2 ASN C 116      83.247 101.707 -13.020  1.00 23.76      C
ATOM   4291  C   ASN C 116      86.139  99.447 -15.378  1.00 27.65      C
ATOM   4292  O   ASN C 116      87.027  99.957 -14.695  1.00 31.18      C
ATOM   4293  N   ASN C 117      86.060  98.132 -15.593  1.00 27.61      C
ATOM   4294  CA  ASN C 117      87.030  97.189 -15.048  1.00 29.18      C
ATOM   4295  CB  ASN C 117      88.475  97.578 -15.449  1.00 27.03      C
ATOM   4296  CG  ASN C 117      88.724  97.389 -16.951  1.00 30.01      C
ATOM   4297  OD1 ASN C 117      87.901  96.793 -17.638  1.00 27.30      C
ATOM   4298  ND2 ASN C 117      89.853  97.883 -17.455  1.00 29.00      C
ATOM   4299  C   ASN C 117      86.958  96.986 -13.543  1.00 31.56      C
ATOM   4300  O   ASN C 117      87.748  96.230 -12.994  1.00 31.15      C
ATOM   4301  N   MET C 118      86.035  97.652 -12.860  1.00 33.87      C
ATOM   4302  CA  MET C 118      85.918  97.430 -11.421  1.00 38.31      C
ATOM   4303  CB  MET C 118      85.431  98.700 -10.723  1.00 43.16      C
ATOM   4304  CG  MET C 118      86.446  99.857 -10.744  1.00 53.52      C
ATOM   4305  SD  MET C 118      85.763 101.385 -10.037  1.00 58.36      C
ATOM   4306  CE  MET C 118      86.038 101.027  -8.271  1.00 63.17      C
ATOM   4307  C   MET C 118      84.937  96.281 -11.182  1.00 41.22      C
ATOM   4308  O   MET C 118      84.034  96.039 -12.001  1.00 39.23      C
ATOM   4309  N   TRP C 119      85.108  95.588 -10.058  1.00 39.36      C
ATOM   4310  CA  TRP C 119      84.276  94.458  -9.706  1.00 34.52      C
ATOM   4311  CB  TRP C 119      85.044  93.494  -8.830  1.00 37.83      C
ATOM   4312  CG  TRP C 119      85.916  92.608  -9.625  1.00 34.11      C
ATOM   4313  CD2 TRP C 119      85.497  91.515 -10.449  1.00 33.34      C
ATOM   4314  CE2 TRP C 119      86.652  90.975 -11.053  1.00 32.21      C
ATOM   4315  CE3 TRP C 119      84.250  90.935 -10.741  1.00 29.94      C
ATOM   4316  CD1 TRP C 119      87.264  92.691  -9.755  1.00 31.13      C
ATOM   4317  NE1 TRP C 119      87.721  91.715 -10.608  1.00 36.30      C
ATOM   4318  CZ2 TRP C 119      86.610  89.897 -11.919  1.00 29.11      C
ATOM   4319  CZ3 TRP C 119      84.206  89.869 -11.594  1.00 31.88      C
ATOM   4320  CH2 TRP C 119      85.384  89.352 -12.181  1.00 32.92      C
ATOM   4321  C   TRP C 119      82.930  94.725  -9.066  1.00 45.62      C
ATOM   4322  O   TRP C 119      82.742  95.703  -8.345  1.00 44.53      C
ATOM   4323  N   GLY C 120      82.022  93.799  -9.399  1.00 52.00      C
ATOM   4324  CA  GLY C 120      80.621  93.709  -8.986  1.00 49.40      C
ATOM   4325  C   GLY C 120      79.864  94.960  -8.669  1.00 50.22      C
ATOM   4326  O   GLY C 120      80.454  96.037  -8.703  1.00 53.01      C
ATOM   4327  N   PRO C 121      78.546  94.853  -8.388  1.00 42.28      C
ATOM   4328  CD  PRO C 121      77.760  93.635  -8.569  1.00 46.84      C
ATOM   4329  CA  PRO C 121      77.673  95.988  -8.042  1.00 46.16      C
ATOM   4330  CB  PRO C 121      76.263  95.395  -8.040  1.00 42.57      C
ATOM   4331  CG  PRO C 121      76.380  94.189  -8.846  1.00 45.38      C
ATOM   4332  C   PRO C 121      78.054  96.442  -6.637  1.00 48.37      C
ATOM   4333  O   PRO C 121      78.006  97.631  -6.340  1.00 49.57      C
ATOM   4334  N   THR C 122      78.361  95.485  -5.766  1.00 45.65      C
ATOM   4335  CA  THR C 122      78.735  95.807  -4.388  1.00 48.81      C
ATOM   4336  CB  THR C 122      78.209  94.712  -3.397  1.00 52.33      C
ATOM   4337  OG1 THR C 122      76.777  94.615  -3.488  1.00 54.63      C
ATOM   4338  CG2 THR C 122      78.563  95.064  -1.953  1.00 54.73      C
ATOM   4339  C   THR C 122      80.264  95.881  -4.287  1.00 51.31      C
ATOM   4340  O   THR C 122      80.964  95.769  -5.277  1.00 49.95      C
ATOM   4341  N   ARG C 123      80.792  96.106  -3.094  1.00 56.40      C
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ATOM	4342	CA	ARG	C	123	82.233	96.099	-2.936	1.00	54.17	C
ATOM	4343	CB	ARG	C	123	82.628	96.777	-1.621	1.00	62.98	C
ATOM	4344	CG	ARG	C	123	82.258	98.275	-1.561	1.00	73.33	C
ATOM	4345	CD	ARG	C	123	82.868	98.987	-0.336	1.00	77.96	C
ATOM	4346	NE	ARG	C	123	83.433	100.279	-0.674	1.00	80.89	C
ATOM	4347	CZ	ARG	C	123	84.553	100.439	-1.458	1.00	80.79	C
ATOM	4348	NH1	ARG	C	123	85.166	99.392	-2.007	1.00	79.18	C
ATOM	4349	NH2	ARG	C	123	85.035	101.656	-1.696	1.00	81.16	C
ATOM	4350	C	ARG	C	123	82.566	94.608	-2.890	1.00	52.07	C
ATOM	4351	O	ARG	C	123	81.687	93.780	-2.609	1.00	51.24	C
ATOM	4352	N	LEU	C	124	83.401	94.245	-3.210	1.00	46.24	C
ATOM	4353	CA	LEU	C	124	84.175	92.836	-3.137	1.00	43.03	C
ATOM	4354	CB	LEU	C	124	85.682	92.655	-3.342	1.00	38.28	C
ATOM	4355	CG	LEU	C	124	86.181	92.386	-4.766	1.00	39.78	C
ATOM	4356	CD1	LEU	C	124	87.714	92.314	-4.721	1.00	41.84	C
ATOM	4357	CD2	LEU	C	124	85.591	91.090	-5.304	0.00	41.07	C
ATOM	4358	C	LEU	C	124	83.395	92.371	-1.738	1.00	35.52	C
ATOM	4359	O	LEU	C	124	83.740	93.175	-0.807	1.00	32.32	C
ATOM	4360	N	PRO	C	125	83.473	91.080	-1.574	1.00	31.53	C
ATOM	4361	CD	PRO	C	125	83.668	89.969	-2.523	1.00	35.48	C
ATOM	4362	CA	PRO	C	125	83.093	90.568	-0.255	1.00	36.74	C
ATOM	4363	CB	PRO	C	125	82.668	89.127	-0.554	1.00	32.42	C
ATOM	4364	CG	PRO	C	125	83.629	88.741	-1.610	1.00	33.06	C
ATOM	4365	C	PRO	C	125	84.328	90.593	0.623	1.00	36.97	C
ATOM	4366	O	PRO	C	125	85.438	90.594	0.117	1.00	34.38	C
ATOM	4367	N	THR	C	126	84.130	90.571	1.930	1.00	41.39	C
ATOM	4368	CA	THR	C	126	85.039	90.584	2.857	1.00	44.67	C
ATOM	4369	CB	THR	C	126	85.171	91.881	3.691	1.00	49.35	C
ATOM	4370	OG1	THR	C	126	86.470	92.211	4.174	1.00	58.86	C
ATOM	4371	CG2	THR	C	126	84.227	91.731	4.855	1.00	46.39	C
ATOM	4372	C	THR	C	126	85.179	89.343	3.765	1.00	43.43	C
ATOM	4373	O	THR	C	126	84.191	88.820	4.068	1.00	41.61	C
ATOM	4374	N	CYS	C	127	86.333	88.832	4.164	1.00	46.42	C
ATOM	4375	CA	CYS	C	127	86.548	87.679	5.068	1.00	46.58	C
ATOM	4376	C	CYS	C	127	86.997	88.162	6.361	1.00	47.12	C
ATOM	4377	O	CYS	C	127	88.182	88.490	6.384	1.00	44.98	C
ATOM	4378	CB	CYS	C	127	87.153	86.515	4.485	1.00	41.09	C
ATOM	4379	SG	CYS	C	127	86.397	85.611	3.072	1.00	36.94	C
ATOM	4380	N	VAL	C	128	86.202	88.224	7.422	1.00	47.64	C
ATOM	4381	CA	VAL	C	128	86.671	88.675	8.725	1.00	50.09	C
ATOM	4382	CB	VAL	C	128	85.674	89.670	9.349	1.00	53.76	C
ATOM	4383	CG1	VAL	C	128	84.322	88.993	9.553	1.00	56.55	C
ATOM	4384	CG2	VAL	C	128	86.211	90.180	10.678	1.00	55.81	C
ATOM	4385	C	VAL	C	128	86.860	87.494	9.696	1.00	50.97	C
ATOM	4386	O	VAL	C	128	86.117	86.494	9.653	1.00	47.21	C
ATOM	4387	N	SER	C	129	87.860	87.611	10.563	1.00	44.79	C
ATOM	4388	CA	SER	C	129	88.146	86.561	11.534	1.00	41.23	C
ATOM	4389	CB	SER	C	129	89.073	86.901	12.370	1.00	36.76	C
ATOM	4390	OG	SER	C	129	89.493	85.755	13.423	1.00	38.45	C
ATOM	4391	C	SER	C	129	87.020	86.289	12.506	1.00	42.12	C
ATOM	4392	O	SER	C	129	86.396	87.214	13.030	1.00	38.42	C
ATOM	4393	N	VAL	C	130	86.733	85.004	12.747	1.00	42.88	C
ATOM	4394	CA	VAL	C	130	85.786	84.566	13.712	1.00	48.17	C
ATOM	4395	CB	VAL	C	130	85.679	83.028	13.724	1.00	49.37	C
ATOM	4396	CG1	VAL	C	130	85.006	82.570	15.003	1.00	55.87	C

ATOM	4397	CG2	VAL	C	130	84.879	82.558	12.510	1.00	47.26	C
ATOM	4398	C	VAL	C	130	86.191	85.042	15.124	1.00	47.25	C
ATOM	4399	O	VAL	C	130	85.334	85.271	15.976	1.00	49.24	C
ATOM	4400	N	PHE	C	131	87.495	85.202	15.360	1.00	42.64	C
ATOM	4401	CA	PHE	C	131	87.979	85.639	16.665	1.00	43.25	C
ATOM	4402	CB	PHE	C	131	89.429	85.174	16.873	1.00	37.67	C
ATOM	4403	CG	PHE	C	131	89.608	83.691	16.666	1.00	36.56	C
ATOM	4404	CD1	PHE	C	131	90.324	83.218	15.589	1.00	30.51	C
ATOM	4405	CD2	PHE	C	131	88.927	82.770	17.461	1.00	32.59	C
ATOM	4406	CE1	PHE	C	131	90.357	81.848	15.278	1.00	32.11	C
ATOM	4407	CE2	PHE	C	131	88.955	81.399	17.157	1.00	37.78	C
ATOM	4408	CZ	PHE	C	131	89.674	80.938	16.055	1.00	33.91	C
ATOM	4409	C	PHE	C	131	87.849	87.146	16.797	1.00	45.03	C
ATOM	4410	O	PHE	C	131	88.533	87.896	16.104	1.00	43.08	C
ATOM	4411	N	PRO	C	132	86.980	87.606	17.719	1.00	49.31	C
ATOM	4412	CD	PRO	C	132	86.384	86.810	18.806	1.00	48.64	C
ATOM	4413	CA	PRO	C	132	86.730	89.029	17.954	1.00	51.76	C
ATOM	4414	CB	PRO	C	132	85.882	88.026	19.227	1.00	51.00	C
ATOM	4415	CG	PRO	C	132	86.345	87.802	19.927	1.00	49.99	C
ATOM	4416	C	PRO	C	132	87.948	89.921	18.054	1.00	54.56	C
ATOM	4417	O	PRO	C	132	88.018	90.941	17.371	1.00	59.16	C
ATOM	4418	N	LEU	C	133	88.913	89.558	18.887	1.00	53.87	C
ATOM	4419	CA	LEU	C	133	90.089	90.396	18.991	1.00	56.98	C
ATOM	4420	CB	LEU	C	133	90.854	90.093	20.274	1.00	53.54	C
ATOM	4421	CG	LEU	C	133	89.997	90.162	21.538	1.00	52.81	C
ATOM	4422	CD1	LEU	C	133	90.901	90.183	22.748	1.00	53.95	C
ATOM	4423	CD2	LEU	C	133	89.142	91.398	21.540	1.00	53.34	C
ATOM	4424	C	LEU	C	133	90.958	90.156	17.772	1.00	58.59	C
ATOM	4425	O	LEU	C	133	92.106	90.579	17.726	1.00	54.07	C
ATOM	4426	N	GLU	C	134	91.054	89.741	16.857	1.00	60.78	C
ATOM	4427	CA	GLU	C	134	91.010	89.258	15.522	1.00	70.26	C
ATOM	4428	CB	GLU	C	134	91.448	90.184	14.475	1.00	72.39	C
ATOM	4429	CG	GLU	C	134	90.575	91.428	14.421	1.00	75.60	C
ATOM	4430	CD	GLU	C	134	89.133	91.113	14.077	1.00	78.38	C
ATOM	4431	OE1	GLU	C	134	88.819	89.923	13.866	1.00	80.20	C
ATOM	4432	OE2	GLU	C	134	88.317	92.057	14.018	1.00	80.22	C
ATOM	4433	C	GLU	C	134	91.879	87.908	15.438	1.00	71.86	C
ATOM	4434	O	GLU	C	134	92.143	87.521	16.835	1.00	73.34	C
ATOM	4435	OXT	GLU	C	134	92.658	87.662	14.702	1.00	76.05	C
ATOM	4436	C1	NAG	D	1	91.022	77.190	13.373	1.00	39.02	D
ATOM	4437	O1	NAG	D	1	90.217	76.061	13.510	1.00	53.38	D
ATOM	4438	C2	NAG	D	1	92.379	76.764	12.861	1.00	36.79	D
ATOM	4439	N2	NAG	D	1	92.264	76.234	11.516	1.00	39.67	D
ATOM	4440	C7	NAG	D	1	92.851	76.904	10.527	1.00	40.49	D
ATOM	4441	O7	NAG	D	1	93.488	77.963	10.726	1.00	46.19	D
ATOM	4442	C8	NAG	D	1	92.771	76.338	9.115	1.00	36.88	D
ATOM	4443	C3	NAG	D	1	92.972	75.726	13.816	1.00	35.98	D
ATOM	4444	O3	NAG	D	1	94.293	75.444	13.394	1.00	40.30	D
ATOM	4445	C4	NAG	D	1	92.986	76.292	15.264	1.00	37.37	D
ATOM	4446	O4	NAG	D	1	93.308	75.255	16.169	1.00	36.52	D
ATOM	4447	C5	NAG	D	1	91.610	76.877	15.659	1.00	38.38	D
ATOM	4448	O5	NAG	D	1	91.167	77.818	14.663	1.00	39.81	D
ATOM	4449	C6	NAG	D	1	91.599	77.601	16.994	1.00	34.64	D
ATOM	4450	O6	NAG	D	1	92.510	78.695	16.984	1.00	35.80	D
ATOM	4451	C1	NAG	E	1	90.580	70.350	4.612	1.00	80.29	E

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ATOM   4452  O1  NAG E   1      90.608  71.734   4.755  1.00 82.28      E
ATOM   4453  C2  NAG E   1      91.606  69.705   5.560  1.00 79.89      E
ATOM   4454  N2  NAG E   1      91.383  70.221   6.901  1.00 79.48      E
ATOM   4455  C7  NAG E   1      90.709  69.507   7.799  1.00 79.52      E
ATOM   4456  O7  NAG E   1      89.865  68.652   7.495  1.00 78.01      E
ATOM   4457  C8  NAG E   1      91.027  69.791   9.263  1.00 77.64      E
ATOM   4458  C3  NAG E   1      93.061  70.018   5.141  1.00 79.82      E
ATOM   4459  O3  NAG E   1      93.945  69.116   5.805  1.00 80.58      E
ATOM   4460  C4  NAG E   1      93.291  69.924   3.618  1.00 80.30      E
ATOM   4461  O4  NAG E   1      94.526  70.547   3.285  1.00 80.30      E
ATOM   4462  C5  NAG E   1      92.148  70.607   2.853  1.00 80.10      E
ATOM   4463  O5  NAG E   1      90.884  70.035   3.252  1.00 79.60      E
ATOM   4464  C6  NAG E   1      92.253  70.476   1.341  1.00 80.36      E
ATOM   4465  O6  NAG E   1      91.044  70.874   0.705  1.00 78.94      E
END
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While various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications and adaptations are within the scope of the present invention, as set forth in the following claims.